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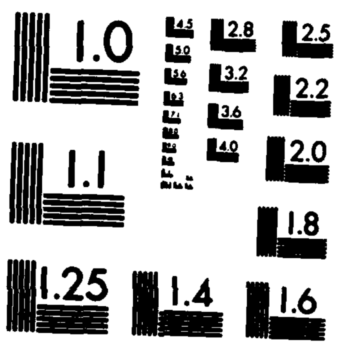

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Final Rpt., 1 July 77 - 31 May '80
Contract DAMD-17-77-C-7040

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MODELING AND SIMULATION OF WASTEWATER REUSE SYSTEMS - DYNAMIC PROCESS SIMULATOR

FINAL REPORT

CECIL L. SMITH, DAVID M. STARKS,
AND WARREN T. ABBOTT

MAY 1982

ARTHUR M. STERLING, FINAL PRINCIPAL INVESTIGATOR

Supported by

U.S. ARMY MEDICAL RESEARCH AND DEVELOPMENT COMMAND
Fort Detrick, Frederick, Maryland 21701

Contract No. DAMD 17-77-C-7040

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SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER	2. GOVT ACCESSION NO.	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) Modeling and Simulation of Wastewater Reuse Systems - Dynamic Process Simulator		5. TYPE OF REPORT & PERIOD COVERED Final Report July 1, 1977 - May 31, 1980
		6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) Cecil L. Smith, David M. Starks, Warren T. Abbott		8. CONTRACT OR GRANT NUMBER(s) DAMD 17-77-C-7040
9. PERFORMING ORGANIZATION NAME AND ADDRESS Department of Chemical Engineering, Louisiana State University, Baton Rouge, LA 70803		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS 62720A.3E162720A835.00.074
11. CONTROLLING OFFICE NAME AND ADDRESS U.S. Army Medical Research & Development Command, Fort Detrick, Frederick, MD 21701		12. REPORT DATE May 1982
		13. NUMBER OF PAGES 184
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)		15. SECURITY CLASS. (of this report) unclassified
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release; distribution unlimited.

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

Final Principal Investigator--Arthur M. Sterling

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Models	Ozonation	Water Reuse
Ultrafiltration	Hyperchlorination	
Reverse Osmosis	Simulation	

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

To aid in the development of the control strategy and the fault detection/fault isolation logic for a self-contained wastewater treatment system, a dynamic model of the system has been developed. The model integrates component models for water processing units into a process simulator to facilitate the simulation of a variety of configurations for water reuse processes. This report describes the simulator modules, the use of the simulator, and the details of input data preparation.

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Executive Summary

For support of field medical units, the U.S. Army is developing a self-contained wastewater treatment system to produce potable water for use within the unit. To aid in developing the control strategy and the fault detection/fault isolation logic, a dynamic model of the system has been developed.

The dynamic model consists of component models for an ultrafiltration unit, a tubular reverse osmosis unit, an ozonation contacting unit, and a hyperchlorination unit. These component models are incorporated into a process simulator to facilitate the simulation of a variety of configurations for water-reuse processes. In addition to the component models, the process simulator includes models for general purpose process elements such as mixed tanks, overflow tanks, pumps, stream splitters, and stream mixers, and general purpose control elements such as sensors, manipulators, binary controllers, ratio controllers, and PID controllers.

To estimate the coefficients in the individual component models, a Pattern Search strategy was used to minimize a cost function which penalized for model deviation from experimental data. Experimental data were obtained first from experiments that formed the basis of the design of a pilot plant version of a water-reuse system and then from the operation of this plot plant.

To make the integrated model as flexible as possible, the plant configuration--the process units, as well as the origin and destination of every stream--is specified by input data. Details on the use of the simulator and the preparation of input data are included in this report.

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Introduction

The U.S. Army has a requirement to provide a mission-oriented medical treatment system which is designed and equipped to facilitate rapid establishment and disestablishment. The flexibility permits immediate response for a medical support unit to any tactical, environmental or geographical change. This system will provde a contamination-free and controlled environment in which medical, surgical and ancillary procedures, and other supporting functions can be performed.

The mobile medical treatment system is termed the MUST Medical Complex. Associated with the MUST Medical Complex is a Water and Waste Management Subsystem (WWMS)*. This subsystem is required to treat and dispose of, without degradation of the environment or danger to personal health, all toxic and contaminated waste materials generated within the functional areas of the Medical Complex. In addition to the waste treatment and disposal, the Water Processing Element (WPE) within the WWMS must be capable of producing potable water from a fresh or brackish water source and nonconsumptive resuse water from the MUST Medical Complex waste water effluent.

The objectives of this program were to:

1. Develop an integrated dynamic model describing the operational characteristics of the water processing element. Emphasis was placed on the reuse mode of operation utilizing the MUST hospital composite waste or the x-ray, laboratory, and OR composite waste. The methodology to apply the model to other configurations and other wastes was also developed.

*The WWMS was deleted from the MUST in 1978.

2. Develop a control/monitoring system for the operation of the WPE, using the dynamic model as the basis.

3. Develop a fault detection/fault isolation package for the WPE, using the dynamic model as the basis.

The first two of the objectives were accomplished, and were incorporated into a simulator program written for a digital computer.

The purpose of this report is to provide an overview of the dynamic process simulator, and to describe the procedures necessary to run the program.

MODELING AND SIMULATION OF WASTEWATER REUSE SYSTEMS - DYNAMIC PROCESS SIMULATOR

1. Overview

The dynamic process simulator is a general purpose computer program. The configuration of the process is specified by the input data, along with the parameters that specify the characteristics of the individual items of equipment in the process. This permits a variety of process configurations to be investigated without requiring any changes in the program source code. While the structure of the simulator is very general, the program has been tailored to meet the needs of the MUST WPE.

2. Streams

For purpose of the simulator, the process is represented by individual pieces of equipment interconnected by process streams. Associated with each stream is a stream vector that specifies the status of the stream. The number of elements in each stream vector is n_s.

The first element in the stream vector is always the flow rate. The remaining elements define the properties of the stream (composition, temperatures, etc.). As presently implemented for the MUST WPE, a stream vector consists of the following:

Element	Definition
1	Flow, m^3/hr
2	Concentration of suspended solids, g/m^3
3	Concentration of dissolved solids, g/m^3
4	Concentration of total organic carbon, (TOC), g/m^3

At some time in the future, it may be necessary to add temperature and/or pressure to this list.

Each stream in the process is designated by a unique number.

3. Process Equipment

For each unit, the following information must be entered:

1. Unit number
2. Equipment type
3. Input streams
4. Output streams
5. Parameters specifying equipment characteristics

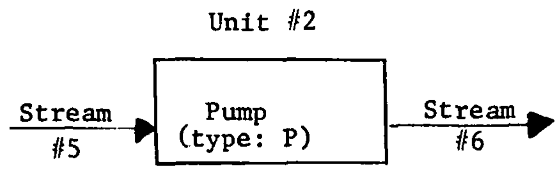
For each unit two data cards must be entered. The first data card specifies the first four items in the above list; the second card specifies the parameters.

For each unit a maximum of five streams may be specified, with any mix of input and output streams. The data required are as follows:

1. Unit number
2. Equipment type
3. Stream 1
4. Stream 2
5. Stream 3
6. Stream 4
7. Stream 5

The data are entered using FORMAT (1X,I4,3X,A2,5I5).

For example, the unit



would be specified by the entry

    2   P   5   -6

By convention, input streams are designated by positive stream numbers and output streams by negative stream numbers. Normally all input streams appear prior to output streams. For certain types of equipment, the order is significant.

The data parameters are also specific to each type of equipment.

The simulator presently recognizes the following types of equipment:

Type	Code
Mixed tank	MT
Overflow tank	ØT
Pump	P
Stream splitter	SP
Stream source	SØ
Stream mixer	SM
Ultrafiltration unit	UF
Gel model UF unit	GM
Reverse Osmosis unit	RØ
Tubular RO unit	TR
UV/oxination unit	UV
Hypochlorination unit	HC
Sink	SK

Other pieces of equipment can be easily added to the simulator.

3.1 Mixed Tank (MT)

The mixed tank is described by a total material balance and three component material balances. The total material balance is:

$$\frac{dV}{dt} = \sum_{\text{input}} F_i - \sum_{\text{output}} F_j$$

where V = volume of liquid in the tank, m^3

F_i = flow rate of input stream, m^3/hr

F_j = flow rate of output stream, m^3/hr

Each component material balance is:

$$\frac{d}{dt}(VC) = \sum_{\text{input}} F_i C_i - \sum_{\text{output}} F_j C_j$$

where C = concentration in the tank, g/m^3

C_i = concentration in input stream, g/m^3

C_j = concentration in output stream, g/m^3

Any combination of input and output streams are permitted. The concentration of all exit streams are the same as the concentration in the tank.

For the mixed tank, the following four parameters are required:

Par 1: Initial volume of liquid in the tank, m^3

Par 2: Initial concentration of suspended solids in the tank, g/m^3

Par 3: Initial concentration of dissolved solids in the tank, g/m^3

Par 4: Initial concentration of TOC in the tank, g/m^3

These parameters are entered via FORMAT (4F10.4).

In the initialization calculations for the mixed tank, the concentrations of all output streams are specified as the initial concentrations in the tank.

3.2 Overflow tank (OT)

The basic equations of the overflow tank are the same as for the mixed tank. However, the first stream must be the overflow stream and is specified as follows:

$$F_1 = F_T \text{ for } 0 < V < V_{max}$$

$$F_1 = \sum_{input} F_i - \sum_{output} F_j \text{ for } V = 0 \text{ or } V = V_{max}$$

where

F_1 = overflow stream flow rate, m^3/hr

F_T = design overflow-rate, m^3/hr

V = volume of liquid in tank, m^3

V_{max} = maximum volume of liquid in tank, m^3

F_i = flow rate of input stream, m^3/hr

F_j = flow rate of output stream, m^3/hr

Both F_T and V_{max} are data parameters.

The following six parameters are required for the overflow tank:

Par 1: Initial volume, m^3

Par 2: Initial concentration of suspended solids, g/m^3

Par 3: Initial concentration of dissolved solids, g/m^3

Par 4: Initial concentration of TOC, g/m^3

Par 5: Design overflow rate, m^3/hr

Par 6: Maximum volume, m^3

These parameters are entered according to FORMAT (6F10.4).

In the initialization calcualtions, the concentration of all output streams are set equal to the initial concentration in the tank. Also, the overflow-rate is set equal to F_T.

3.3 Volumetric Pump (P)

This piece of equipment represents either a constant volume pump or a variable volume pump followed by a flow controller. The first stream must be the input stream; the second must be the output stream.

The basic equation for this pump is as follows:

$$F_1 = F_2 = F_p$$

where F_p = flow rate through pump, m^3/hr

F_1 = flow rate of input stream, m^3/hr

F_2 = flow rate of output stream, m^3/hr

Furthermore, the concentration of the output stream is set equal to the concentration of the input stream.

The only input parameter is F_p, which is entered via FORMAT(F10.4).

The initialization calculations are the same as the normal calculations.

3.4 Stream Splitter (SP)

The purpose of this piece of equipment is to split an input stream into two output streams where the flow rate of one output stream is specified. The streams are specified in the following order:

1. Input stream
2. Output stream where flow is fixed
3. Output stream where flow varies

The flow equation describing this piece of equipment is as follows:

$$F_2 = \begin{cases} F_s \text{ if } F_1 \geq F_s \\ F_1 \text{ if } F_1 < F_s \end{cases}$$

$$F_3 = F_1 - F_2$$

where F_1 = flow rate of input stream, m^3/hr

F_2 = flow rate of first output stream, m^3/hr

F_3 = flow rate of second output stream, m^3/hr

F_s = the design split, m^3/hr

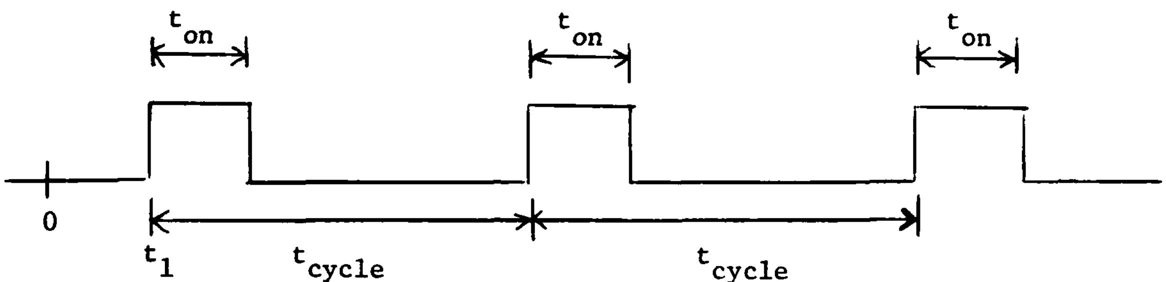
The concentrations in both output streams are set equal to the input concentration.

The only parameter required is F_s, which is entered via FORMAT (F10.4).

The initialization calculations are the same as the normal calculations.

3.5 Stream Source (SO)

The stream source is designed to simulate the pulse-type input streams that are encountered in the MUST hospital. A stream is assumed to behave as follows:



where t_1 = time of start of first pulse, hr.

t_{on} = time duration of pulse, hr.

t_{cycle} = time of cycle, hr

During the flow period, the flow rate and concentration must be specified.

For this unit, the following parameters are required:

Par 1: Time of first pulse, t_1, hr

Par 2: Time duration of pulse, t_{on}, hr

Par 3: Time of cycle, t_{cycle}, hr

Par 4: Flow rate during pulse, m^3/hr

Par 5: Concentration of suspended solids, g/m^3

Par 6: Concentration of dissolved solid, g/m^3

Par 7: Concentration of TOC, g/m^3

These are entered via FORMAT (7F10.4)

The initialization calculations are the same as for the normal calculations.

All input streams must originate with a stream source block.

3.6 Stream Mixer (SM)

The stream mixer is designed to combine up to four input streams to produce a single output stream. In specifying the streams, the output stream must be specified last.

The flow equations describing this unit are as follows:

$$F_j = \sum_{\text{input}} F_i$$

where F_i = flow rate of input stream

F_j = flow rate of output stream

The equation for each concentration is as follows:

$$C_j = \frac{\sum_{\text{input}} F_i C_i}{F_j}$$

where C_i = concentration in input stream

C_j = concentration in output stream

No parameters are required for this unit.

The initialization calculations are the same as the normal calculations.

3.7 Ultrafiltration Unit (UF)

This piece of equipment consists of parallel banks of filtration tubes. The feed stream is forced into one end of the tube bundle, water and dissolved solids are forced through the tubes and collected as the filtered permeate. The concentrate stream is high in suspended solids, and is collected out of the other end of the bundle. In specifying the streams, the permeate stream must be first, the concentrate stream must be second, and the feed stream must be third.

See Starks and Smith (1) and Starks (3) for the model equations.

The parameters required for this unit are:

Par 1: Number of tubes

Par 2: Temperature of feed, °K

Par 3: Pressure drop across the membrane at the inlet, atm

Par 4: Pressure drop down the tubes, atm

Par 5: Diameter of a tube, m

Par 6: Length of a tube, m

These are entered via FORMAT (6F10.4).

The initialization calculations are the same as for the normal calculations.

3.8 Tubular Reverse Osmosis Unit (TR)

This piece of equipment is essentially the same as the ultrafiltration unit, except that the tube diameter is one or two orders of magnitude smaller, and the filtration membrane has smaller pores. These two differences lead to higher rejection of dissolved solids and TOC. See section 3.7 on the UF unit for a definition of the input and output streams.

The parameters required for this unit are the same as for the UF unit given in Section 3.7.

The initialization calculations are the same as for the normal calculations.

3.9 Gel Model Ultrafiltration Unit (GM)

This piece of equipment is essentially the same as the tubular RO unit, except that the boundary layer is assumed to form a gel on the inside surface. This gel increases the rejection of dissolved solids and TOC. See section 3.7 on the UF unit for a definition of the input and output streams.

The parameters required for this unit are the same as for the UF unit given in Section 3.7.

The initialization calculations are the same as for the normal calculations.

3.10 Reverse Osmosis Unit (RO)

This piece of equipment consists of a bundle of tube fibers around a central porous tube. The feed enters the central tube under very high pressure. The contaminated water flows radially around the outside of the fibers, forcing the water to permeate to the inside of the tubes; the fluid in the fibers is collected as the permeate stream. The fluid that reaches the outer region of the bundle is very high in concentration of dissolved solids and TOC and is collected as the concentrate stream. Suspended solids should not be present in the feed. The rejection is very high, but the flow rate is very small. The feed to the RO unit should be the permeate of an ultrafiltration unit, UF, TR, or GM. In specifying the streams, the permeate must be first, the concentrate must be second, the feed must be third.

See Starks and Smith (2) and Starks (3) for the model equations.

The parameters required for this unit are:

Par 1: Pressure drop across the membrane (fiber), atm

Par 2: Temperature of the feed, °K

Par 3: Length of the fibers, m

Par 4: Outer radius of bundle, m

Par 5: Inner radius of bundle, m (center tube outer radius)

Par 6: Diameter of a fiber, m

These are entered via FORMAT (6F10.4).

The initialization calculations are the same as for the normal calculations.

3.11 Ultraviolet/Ozonation Unit (UV)

This piece of equipment is used to oxidize organic compounds by ultraviolet activate ozonation. The contaminated water is simultaneously sparged with ozone and irradiated with ultraviolet light. The unit consists of a precontactor and six contact stages in series. There is one input stream and one output stream. In specifying the streams, the feed stream must be specified first and the effluent (output) stream must be specified second.

See Starks (3) for the model equations.

The parameters required for this unit are:

Par 1: Initial concentration of suspended solids, g/m^3

Par 2: Initial concentration of dissolved solids, g/m^3

Par 3: Initial concentration of TOC, g/m^3

Par 4: Inlet O_3 concentration, moles O_3/mole gas

Par 5: Volumetric gas flow rate, m^3/hr

Par 6: Precontactor flag (0 = No precontactor)

Par 7: Number of stages

Par 8: Area of a contactor, m^2

Par 9: Area of a precontactor, m^2

Par 10: Height of a stage, m

Par 11: Feed temperature, °K

Par 12: Operating pressure, atm

These are entered via FORMAT (12F10.4). Note that two parameter cards are necessary (1-8 on the first, 9-12 on the second).

The initialization calculations are the same as for the normal calculations.

3.12 Hypochlorite Unit (HC)

This piece of equipment is a stirred tank in which calcium hypochlorite $Ca(O\ Cl)_2$ is added to serve as a bacteria retardant. The feed stream must be specified first and the effluent stream must be specified second.

See Starks (3) for the model equations.

The parameters for this unit are:

Par 1: pH of the output

Par 2: Initial chlorite in the HC unit

Par 3: Initial concentration of suspended solids, g/m^3

Par 4: Initial concentration of dissolved solids, g/m^3

Par 5: Initial concentration of TOC, g/m^3

Par 6: Feed rate of calcium hypochlorite, m^3/hr

Par 7: Volume of HC unit, m^3

Par 8: Concentration of $Ca(O\ Cl)_2$, g/m^3

These are entered via FORMAT (8F10.4).

Initialization calculations assume that the hypochlorination tank is filled up to its maximum volume at the concentration of the feed stream.

3.13 Sink (SK)

As indicated earlier, all input streams to the process must originate with the source block. Similarly, all streams leaving the process must be inputs to a block called the "Sink". One reason for this is that each stream must originate with one and only one block and each stream must terminate with one and only one block.

Actually, the sink block plays no role in the simulation. The only calculation procedure involved is that the collective stream flows (total and component) are integrated for the overall material balance calculations.

Each sink block may have up to five input streams. The process configuration may contain multiple sink blocks.

4. Control Elements

For each control element, the following information must be entered:

1. Unit number

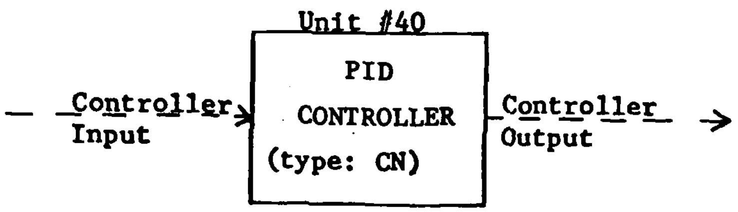
2. Control element type

3. Parameters specifying control element characteristics

As for other units in the simulator, two data cards must be entered for each control element. The first data card specifies items one and two above; the second card specified the parameters.

Unlike the process equipment, there are no input or output streams to be specified. The first card is entered using FORMAT (1X,I4,3X,A2).

For example, the unit



would be specified by the entry

```
    40   CN
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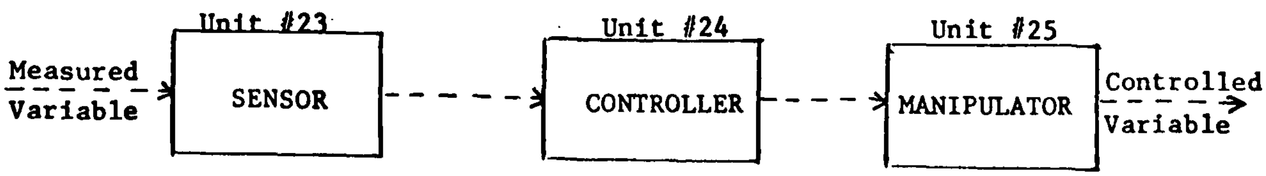
The data parameters are specific to each type of control element. There are three basic control elements: the sensor, the manipulator, and the controller. A control scheme is defined by a unique group of sensor-controller-manipulator arrangement. The unit numbers for each control element in a control scheme must be sequential, starting with the sensor. For example:



The simulator presently recognizes the following types of control elements:

TYPE	CODE
Sensor	SN
Manipulator	MN
Binary Controller	BC
Ratio Controller	RC
PID Controller	CN

4.1 Sensor (SN)

The sensor is used to "measure" (return) the value of either a unit parameter (i.e. volume) or a stream element (flow rate or concentration). The computational equation is:

$$c_n = \frac{1}{\tau} (r - c_{n-1}) \quad \Delta t, \ \tau \neq 0$$

$$c_n = r \qquad\qquad , \ \tau = 0$$

where c_n is the output of the sensor (to the controller)

r is the "reading" or "measured value"

c_{n-1} is the previous output value

τ is the integration time constant, hr

Δt is the integration step size, hr

The parameters required are:

Par 1: Unit number or stream number

Par 2: Parameter or element number

Par 3: Initial output value

Par 4: The integration time constant, τ, hr

These parameters are entered via FORMAT (4I0.4). To specify a unit, enter a negative value; to specify a stream, enter a positive value.

The initialization calculations are the same as the normal calculations.

4.2 Manipulator (MN)

The manipulator is used to change the value of a parameter of a unit (i.e. increase a pump flow rate). The computational equation is:

$$y = \begin{cases} y_{min}, \text{ if } m < y_{min} \\ m, \text{ if } y_{min} \leq m \leq y_{max} \\ y_{max}, \text{ if } m > y_{max} \end{cases}$$

where y is the output value (new parameter value)

m is the signal from the controller

y_{min} is the lower limit of the parameter

y_{max} is the upper limit of the parameter

The parameters required are:

Par 1: Unit number of unit to manipulate (negative)

Par 2: Number of parameter to be manipulated

Par 3: Initial output value

Par 4: Upper limit

Par 5: Lower limit

These parameters are entered via FORMAT (5F10.4).

The initialization calculations are the same as the normal calculations.

4.3 Binary Controller (BC)

This control element represents a binary (on/off) controller. The computational equation is:

if automatic

$$m_n = \begin{cases} m_{min}, & \text{if } c < c_{min} \\ m_{n-1}, & \text{if } c_{min} \leq c \leq c_{max} \\ m_{max}, & \text{if } c > c_{max} \end{cases}$$

if manual

$$m_n = m_{man}$$

where m_n is the controller output

m_{n-1} is the previous value

m_{min} is the lower limit output

m_{max} is the upper limit output

c is the controller input (sensor output)

c_{min} is the lower setpoint

c_{max} is the upper setpoint

The parameters required are:

Par 1: Sensor unit number (negative)

Par 2: Manipulator unit number (negative)

Par 3: Lower setpoint value

Par 4: Upper setpoint value

Par 5: Initial output value

Par 6: Upper limit output value

Par 7: Lower limit output value

Par 8: Operation mode (negative = Automatic, positive = value for Manual)

These parameters are entered via FORMAT (8F10.4), note that two data cards are required.

The initialization calculations are the same as the normal calculations.

4.4 Ratio Controller (RC)

This control element represents a ratio controller. The computational equation is

$$m = \begin{cases} r\ c, & \text{if automatic} \\ m_{man}, & \text{if manual} \end{cases}$$

where m is the controller output value

r is the ratio (output/input)

c is the controller input (sensor output)

m_{man} is the output value for manual

The parameters required are

Par 1: Unit number of sensor (negative)

Par 2: Unit number of manipulator (negative)

Par 3: Ratio

Par 4: Operation mode (negative = Automatic, positive = value for Manual)

These parameters are entered via FORMAT (4F10.4).

The initialization calculations are the same as the normal calculations.

4.5 PID Controller (CN)

This control element represent a three mode, proportional-integral-derivative, controller. The computational equation is the velocity algorithm:

$$e_i = r - c_i$$

$$\frac{d\,e_i}{dt} = \frac{1}{\Delta t}\,(e_i - e_{i-1})$$

$$\frac{d^2 e_i}{dt^2} = \frac{1}{(\Delta t)^2}\,(e_i - 2\,e_{i-1} + e_{i-2})$$

$$\Delta m_i = K_c \left(\frac{d\,e_i}{dt} + \frac{1}{T_I}\,e_i + T_D\,\frac{d^2 e}{dt^2} \right)$$

$$m_{i+1} = \begin{cases} m_i + \Delta m_i\,\Delta t, & \text{if automatic} \\ m_{man}, & \text{if manual} \end{cases}$$

where r is the set point value

c_i is the measured variable

e_i is the error in the signal

Δt is the integration step size

m_i is the controller signal

K_c is the controller gain

T_I is the reset time constant, hr

T_D is the derivative time constant, hr

m_{man} is the output value for manual

The parameters required are:

Par 1: Sensor unit number (negative)

Par 2: Manipulator unit number (negative)

Par 3: Setpoint

Par 4: Gain, K_c

Par 5: Reset time constant, hr

Par 6: Derivative time constant, hr

Par 7: Operation mode (negative = Automatic, positive = value for Manual)

These parameters are entered via FORMAT (7F10.4).

The initialization calculations are the same as the normal calculations.

5. Data Preparation

The input data cards provide for the entry of the following types of information.

1. Model parameters such as kinetic parameters, mass transfer coefficients, etc.
2. Specification of the plant itself, including
   a. Configuration (equipment and streams)
   b. Design parameters
   c. Initial conditions
3. Descriptions, including
   a. Equipment names
   b. Names for equipment parameters
   c. Stream names
   d. Names for stream elements
4. Run control parameters (time of run, integration interval)
5. Variables to be printed, which may be either
   a. Any element of any stream (e.g., flow rate of stream 5)
   b. Any parameter associated with any unit (e.g., Volume of liquid in unit 8)
6. Plot control information, including
   a. Variables to be plotted
   b. Time of plot
   c. Arrangement of graphs
7. Variables to be save on an offline storage medium, which may be either
   a. Any element of any stream
   b. Any parameter associated with any unit
8. Retrieval of variables from a previous run saved on offline storage.

As the data are entered, checks are made to assure that the data are meaningful.

To assist in the preparation of a data deck, data control cards are used to establish segments in the data deck. The first and last cards in each segment are data control cards. The data control card that appears at the beginning of the segment consists of an asterisk (*) in column 1 followed by up to three characters that identify the segment. The data control card at the end of the segment consists only of an asterisk (*) in column 1.

Table 5.1 lists the nine segments and specifies the data control cards for each. The general layout of the data deck is given in Figure 5.1. The following sections describe each segment in more detail.

Table 5.1. Segment Definitions

Segment	Data Control Card	Segment Required/ Optional	Purpose of Segment
Model Parameters	*MP	Optional	Used to read any model parameters required for modules such as UF, RO, etc.
Stream Elements	*SE	Required	Reads engineering units and description for each stream element
Stream Names	*SN	Optional	Reads description for each stream
Configuration	*C	Required	Reads plant configuration
Print Definition	*PR	Required	Reads specifications for variables to be printed
Plot Definition	*PL	Optional	Reads specifications for variables to be plotted
Run	*RUN	Required	Reads execution control parameters and initiates simulation
Plot Control	*PC	Required when *PT used	Reads control information for generating plots
Off-line storage	*OF	Optional	Reads specifications for variables to be save on an off-line storage device (i.e. disk or tape)
Old values	*OL	Optional	To be used in place of RUN. To retrieve values of a previous run that were saved on an off-line storage device

```
*MP
  {model parameters}
*
*SE
  {stream element definitions}
*
*SN
  {stream descriptions}
*
*C
  {plant configuration}
*
*OF
  {off-line variable definitions}
*
*PR
  {print variable definitions}
*
*PL
  {plot variable definitions}
*
*PC
  {plot control information}
*
*OL
  {old value definitions}
*
*RUN
  {run time and integration size}
*
```

Figure 5.1. Data deck

5.1 Model Parameters (*MP)

For modules such as UF, RO, etc., the model parameters are determined by fitting the model to experimental data. Thus, it is necessary to provide a facility whereby these parameters can be easily changed. Four options are available:

1. Within the subroutine for each respective module, use DATA statements to specify the model parameters. This is acceptable only if the primary subroutine does not call additional subroutines that require the model parameters.
2. Put all model parameters into a labeled COMMON statement, and then use DATA statements in the BLOCK DATA subprogram to initialize the parameters.
3. Put all model parameters into a labeled COMMON statement, and then read the values of the model parameters from data cards.
4. A combination of options 2 and 3. A set of model parameters are initialized in the BLOCK DATA subprogram. Different values may be entered through the use of NAMELIST statements.

The model parameter (*MP) segment of the data deck uses option 4.

Upon encountering the *MP data control card, the program calls subroutine RMODPR. This subroutine consists of statements such as

```
READ (5,NAMERO)
```

NAMERO is the name of a NAMELIST block for model parameters for the RO model. Any, all, or none of the NAMELIST parameters may be specified. These parameters are contained in labeled COMMON statements that also appear in the subroutines in which the values of the parameters are needed.

Parameters to be modified are specified as follows:

```
XX
 &NAMEXX
 A = x, B = y,
 C = z
 &END
```

where XX is the two character code of the desired module, i.e. UF, RO

A,B,C, etc. are the names of the parameters of XX to be changed

x,y,z, etc. are the corresponding numeric values

The user of the simulator can readily add parameters, delete parameters, and make any other changes required to meet the needs of the respective module for which the parameters are being read. Figure 5.2 gives the listing for RMODPR for reading the parameters for the ultrafiltration module only. Figure 5.3 lists the *MP segment of the data deck, and Figure 5.4 gives the corresponding output listing. The parameters are written from RMODPR so that errors may readily be detected, and so that outputs of runs using different values may be identified.

If no model parameters are to be changed from the default values, then the *MP section may be omitted. In this case, no parameters are changed or printed out. If it is desired to have a list of all of the default values, then enter

```
*MP
NONE
*
```

```
      SUBROUTINE RMODPR
C
C  READ MODEL PARAMETERS
C
      REAL MWHOCL, MWOCL, L, NF, NTPIDT, KLA, KHENRY, KRATE,
     &     KDCOMP
      REAL*8 VHC, ALPHC, RDHC, KEQHC, CAOCL2, DTHC
C  LABELED COMMON STATEMENTS FOR REVERSE-OSMOSIS UNITS
      COMMON /REVOS1/ L, FLOW, RO, RI, DR, DP, DELP, RHOB,
     &                TOLMX, TOLMN
      COMMON /ROFIT / AKA, AKC, ERE, APIRO, BPIRO, GAMARO,
     &                BRO, CRO, NF,ROKE
      COMMON /GFPARM/ TEMP, VISC, MCNT2, MCNT3, JWRITE
      COMMON /REVOS2/ KWRITE, NSTEPS
C  LABELED COMMON STATEMENTS FOR OZONE UNITS
      COMMON /STAGES/ NSTAGE, PRECON
      COMMON /OZFIT/  KHENRY, ECOZ, ETOC, KRATE, KDCOMP,
     &                EOZD, UVEFCT, ALPHA, EN, QPRIME
      COMMON /OZOPER/ CAREA, PAREA, UVH, UVRHO, UVPRES,
     &                UVTEMP, NWRITE
      COMMON /GASLAW/ RGAS
C  LABELED COMMON STATEMENTS FOR ULTRAFILTRATION MODULE
      COMMON /UFPARM/ PLENUF, DTUBUF, NTUF, JPUFSS, JWUFSS
      COMMON /PARMUF/ TEMPUF, VISCUF, DENBUF, ZREOUF, DROPUF
      COMMON /UFSAV1/ NSTPUF
      COMMON /UFFIT / G1UF, G2UF, GINFUF, C1, C2, CINF
C  LABELED COMMON STATEMENTS FOR TUBULAR R-O MODULE
      COMMON /TRPARM/ PLENTR, DTUBTR, NTTR, JPTRSS, JWTRSS
      COMMON /PARMTR/ TEMPTR, VISCTR, DENBTR, ZEROTR, DROPTR
      COMMON /TRFIT/  G1TR, G2TR, GINFTR, APITR, BTR, CTR,
     &                DCXTR, ADAXTR, BDAXTR, CDAXTR
C  LABELED COMMON STATEMENTS FOR GEL-MODEL
      COMMON /GMPARM/ PLENGM, DTUBGM, NTGM, JPGMSS, JWGMSS
      COMMON /PARMGM/ TEMPGM, VISCGM, DENBGM, ZEROGM, DROPGM
      COMMON /GMFIT/  GAMMA, APIGM, BPIGM, BGM, CGM, RATIO,
     &                DCXGM, ADAXGM, BDAXGM, CDAXGM, CAGEL
C  LABELED COMMON STATEMENTS FOR HYPOCHLORINATION MODULE
      COMMON /HCOPER/ VHC, ALPHC, RDHC, KEQHC, JWRTHC,
     &                MCNTHC, CAOCL2, DTHC
      COMMON /HCSAV2/ MWHOCL, MWOCL, HCRHO
      DIMENSION JCARD(20), IUNIT(8)
      NAMELIST /NAMERO/ TOLMX, TOLMN, MCNT2, MCNT3, KWRITE,
     &                  AKA, AKC, ERE, APIRO, BPIRO, GAMARO,
     &                  BRO, CRO, NF, ROKE, JWRITE, NSTEPS
      NAMELIST /NAMEUV/ KHENRY, ECOZ, ETOC, KRATE, KDCOMP,
     &                  EOZD, UVEFCT, ALPHA, EN, QPRIME,
     &                  NWRITE, RGAS
      NAMELIST /NAMEUF/ JPUFSS, JWUFSS, G1UF, G2UF, GINFUF,
     &                  C1, C2, CINF, PERMIC
      NAMELIST /NAMETR/ JPTRSS, JWTRSS, G1TR, G2TR, GINFTR,
     &                  APITR, BTR, CTR, DCXTR, ADAXTR,
     &                  BDAXTR, CDAXTR
      NAMELIST /NAMEGM/ JPGMSS, JWGMSS, GAMMA, APIGM, BPIGM,
```

Figure 5.2. Listing for RMODPR for reading ultrafiltration model parameters

```
     &                    BGM, CGM, RATIO, DCXGM, ADAXGM,
     &                    BDAXGM, CDAXGM, CAGEL
      NAMELIST /NAMEHC/ VHC, ALPHC, RDHC, KEQHC, JWRTHC,
     &                    MCNTHC, CAOCL2, MWHOCL, MWOCL, HCRHO
      DATA IUNIT/'NONE','*','UF','TR','GM','RO','UV','HC'/
   10 READ(5,20) ICARD,JCARD
   20 FORMAT(A4,T1,20A4)
      DO 30 I=1,8
      IF(ICARD .EQ. IUNIT(I))
     & GO TO (10, 110, 50, 60, 70, 80, 90, 100),I
C           NONE  *   UF  TR  GM  RO  UV   HC
   30 CONTINUE
      WRITE(6,40) JCARD
   40 FORMAT('THE FOLLOWING CARD IS INVALID AND WILL BE',
     & ' IGNORED'/1X,20A4)
      GO TO 10
   50 READ(5,NAMEUF)
      GO TO 10
   60 READ(5,NAMETR)
      GO TO 10
   70 READ(5,NAMEGM)
      GO TO 10
   80 READ(5,NAMERO)
      GO TO 10
   90 READ(5,NAMEUV)
      GO TO 10
  100 READ(5,NAMEHC)
      GO TO 10
  110 WRITE(6,120)
  120 FORMAT('1*MP      MODEL PARAMETERS'/)
C
      WRITE(6,130)
  130 FORMAT('OMODEL PARAMETERS FOR ULTRAFILTRATION MODULE')
      ICARD=0
      WRITE(6,140) JPUFSS, G1UF, G2UF, GINFUF, JWUFSS, C1,
     &             C2, CINF
  140 FORMAT('OJPUFSS=',I3,'    G1UF=',G12.5,'    G2UF=',
     &G12.5,'  GINFUF=',G12.5/'  JWUFSS=',I3,6X,'      C1=',
     &'      C1=',G12.5,'      C2=',G12.5,'    CINF=',G12.5)
C
      WRITE(6,150)
  150 FORMAT('OMODEL PARAMETERS FOR TUBULAR RO MODULE')
      WRITE(6,160) JPTRSS, G1TR, G2TR, GINFTR,JWTRSS,ADAXTR,
     &             BDAXTR, CDAXTR, APITR, BTR, CTR, DCXTR
  160 FORMAT('OJPTRSS=',I3,'    G1TR=',G12.5,'    G2TR=',
     &G12.5,'  GINFTR=',G12.5/'  JWTRSS=',I3,'  ADAXTR=',
     & G12.5,'  BDAXTR=',G12.5,'  CDAXTR=',G12.5/14X,
     & 'APITR=',G12.5,'     BTR=',G12.5,'     CTR=',G12.5/
     & 14X,'DCXTR=',G12.5)
C
      WRITE(6,170)
  170 FORMAT('OMODEL PARAMETERS FOR GEL-MODEL')
      WRITE(6,180) JPGMSS, GAMMA, APIGM, BPIGM, JWGMSS, BGM,
     &             CGM, RATIO, DCXGM, ADAXGM, BDAXGM,
```

Figure 5.2. (continued)

```
     &                  CDAXGM, CAGEL
 180 FORMAT('0JPGMSS=',I3,'   GAMMA=',G12.5,'   APIGM=',
     & G12.5,'    BPIGM=',G12.5/'  JWGMSS=',I3,'     BGM=',
     & G12.5,'      CGM=',G12.5,'    RATIO=',G12.5/14X,
     & 'DCXGM=',G12.5,'  ADAXGM=',G12.5,'  BDAXGM=',G12.5/
     &   12X,'  CDAXGM=',G12.5,'    CAGEL=',G12.5)
C
      WRITE(6,190)
 190 FORMAT('0MODEL PARAMETERS FOR REVERSE OSMOSIS')
      WRITE(6,200) JWRITE, TOLMX, TOLMN, AKA, MCNT2, AKC,
     &             ERE, APIRO, MCNT3, BPIRO, GAMARO, BRO,
     &             NSTEPS, CRO, JWRITE, NF, ROKE
 200 FORMAT('0JWRITE=',I3,'   TOLMX=',G12.5,'   TOLMN=',
     & G12.5,'      AKA=',G12.5/'   MCNT2=',I3,'      AKC=',
     &G12.5,'      ERE=',G12.5,'   APIRO=',G12.5/'   MCNT3=',
     & I3,'   BPIRO=',G12.5,'  GAMARO=',G12.5,'      BRO=',
     & G12.5/'  NSTEPS=',I3,'      CRO=',G12.5,'       NF=',
     & G12.5,'     ROKE=',G12.5)
C
      WRITE(6,210)
 210 FORMAT('0MODEL PARAMETERS FOR THE UV/OZONATION UNIT')
      WRITE(6,220) NWRITE, KHENRY, ECOZ, ETOC, KRATE,
     &             KDCOMP, EOZD, UVEFCT, ALPHA, EN, QPRIME,
     &             RGAS
 220 FORMAT('0NWRITE=',I3,'  KHENRY=',G12.5,'     ECOZ=',
     & G12.5,'     ETOC=',G12.5/14X,'KRATE=',G12.5,
     & '  KDCOMP=',G12.5,'     EOZD=',G12.5/14X,'UVEFCT=',
     & G12.5,'    ALPHA=',G12.5,'       EN=',G12.5/14X,
     & 'QPRIME=',G12.5,'     RGAS=',G12.5)
C
      WRITE(6,230)
 230 FORMAT('0MODEL PARAMETERS FOR HYPOCHLORINATION UNIT')
      WRITE(6,240) JWRTHC, VHC, ALPHC, RDHC, MCNTHC, KEQHC,
     &             CAOCL2, MWHOCL, MWOCL, HCRHO
 240 FORMAT('0JWRTHC=',I3,'       VHC=',G12.5,'    ALPHC=',
     & G12.5,'     RDHC=',G12.5/'  MCNTHC=',I3,'    KEQHC=',
     & G12.5,'  CAOCL2=',G12.5,'  MWHOCL=',G12.5/14X,
     & 'MWOCL=',G12.5,'    HCRHO=',G12.5)
      RETURN
      END
```

Figure 5.2. (continued)

```
*MP
RO
 &NAMERO
 MCNT2=15,
 MCNT3=15,
 &END
*
```

Figure 5.3. Sample data for the *MP data segment.

```
*MP        MODEL PARAMETERS


MODEL PARAMETERS FOR ULTRAFILTRATION MODULE

 JPUFSS=  0      G1UF=  71251.          G2UF=  .40141       GINFUF=  .14674E-03
 JWUFSS=  0        C1=  .10537            C2=  1.1185         CINF=  .46156E-02
               VISCUF=  .32740E-02   DENBUF=  .10000E+07

MODEL PARAMETERS FOR TUBULAR RO MODULE

 JPTRSS=  0      G1TR=  19100.          G2TR=  .57895       GINFTR=  14400.
 JWTRSS=  0   ADAXTR=  .30254E-06   BDAXTR=  .48540E-05   CDAXTR=  .61405
                APITR=  .10391E-07      BTR=  .39526E-04      CTR=  .42112E-02
                DCXTR=  .48000E-01   VISCTR=  .32740E-02   DENBTR=  .10000E+07

MODEL PARAMETERS FOR GEL-MODEL

 JPGMSS=  0     GAMMA=  .0             APIGM=  .0            BPIGM=  .0
 JWGMSS=  0       BGM=  .0               CGM=  .0            RATIO=  .0
                DCXGM=  .0            ADAXGM=  .0           BDAXGM=  .0
               CDAXGM=  .0             CAGEL=  .0           VISCGM=  .32740E-02
               DENBGM=  .10000E+07

MODEL PARAMETERS FOR REVERSE OSMOSIS

 JWRITE=  0     TOLMX=  .50000E-01     TOLMN=  .10000E-01      AKA=  .21170E-01
 MCNT2= 15        AKC=  .57434E-03       ERE=  3.7910        APIRO=  .25260E-06
 MCNT3= 15      BPIRO=  .68100E-04    GAMABO=  18.350          BRO=  .24880E-05
 NSTEPS= 10       CRO=  .13510E-05        NF=  .36940E+08     ROKE=  .62950
 KWRITE=  0      VISC=  .32740E-02     RHOB=  .10000E+07

MODEL PARAMETERS FOR THE UV/OZONATION UNIT

 NWRITE=  0    KHENRY=  .28560E+07      ECOZ=  1.0000         ETOC=  4.1250
                KRATE=  931.24        KDCOMP=  .0             EOZD=  1.0000
               UVEFCT=  .0             ALPHA=  .16667E-03       EN=  .0
               QPRIME=  16830.          RGAS=  .82050        UVRHO=  55.556

MODEL PARAMETERS FOR HYPOCHLORINATION UNIT

 JWRTHC=  0     ALPHC=  .0              RDHC=  .0            MCRHO=  .10000E+07
 MCNTHC= 30     KEQHC=  .27000D-07    CAOCL2=  .0           MWHOCL=  52500.
                MWOCL=  52500.
```

Figure 5.4. Output for reading of the ultrafiltration model parameters

5.2 Stream Elements (*SE)

The purpose of this data segment is to read the engineering units and the descriptions of all elements of the stream vector.

The information for each stream element is punched on a card as follows:

Quantity	Columns	Format
Stream element number	2-5	I4
Engineering units	7-10	A4
Description	16-35	5A4

The cards must be entered in ascending order of the stream element numbers, and a card must be provided for each stream element.

Figure 5.5 lists the *SE segment of the data deck for defining three stream elements. Figure 5.6 gives the corresponding output.

```
*SE
     1 M3/H      FLOW RATE
     2 G/M3      SUSPENDED SOLIDS
     3 G/M3      DISSOLVED SOLIDS
     4 G/M3      TOT. ORG CARBON
*
```

Figure 5.5. Listing of the *SE data segment.

```
*SE      STREAM ELEMENT DEFINITIONS

      ELEMENT   UNITS       DESCRIPTION
         1      M3/H      FLOW RATE
         2      G/M3      SUSPENDED SOLIDS
         3      G/M3      DISSOLVED SOLIDS
         4      G/M3      TOT. ORG CARBON
```

Figure 5.6. Output from the data in Figure 5.5.

5.3 Stream Names (*SN)

The simulator provides for the association of a twenty-character descriptor with each process stream.

The descriptors are entered in the *SN data segment. The format of each card is as follows:

Quantity	Columns	Format
Stream number	2-5	I4
Description	11-30	5A4

The stream numbers may be entered in any order. It is not necessary that a descriptor be entered for each process stream.

Figure 5.7 lists the *SN data segment in which descriptions are provided for ten process streams. The corresponding output is given in Figure 5.8.

In the output generated from other sections of the simulator, the stream descriptor normally accompanies the stream number whenever sufficient space is available.

```
*SN
     1      LABORATORY WASTE
     2      X-RAY WASTE
     3      BAD ACTOR FLOW
     4      OPERATING ROOM WASTE
     5      EQUILIZATION TK DISC
     6      EQ TK PUMP DISCHARGE
     7      RECYCLE FROM UF
     8      UF FEED PUMP SUCTION
     9      UF MODULE FEED FLOW
    10      UF PERMEATE FLOW
*
```

Figure 5.7. Listing of the *SN segment of the data deck.

```
*SN       STREAM NAMES

        STREAM     DESCRIPTION
           1       LABORATORY WASTE
           2       X-RAY WASTE
           3       BAD ACTOR FLOW
           4       OPERATING ROOM WASTE
           5       EQUILIZATION TK DISC
           6       EQ TK PUMP DISCHARGE
           7       RECYCLE FROM UF
           8       UF FEED PUMP SUCTION
           9       UF MODULE FEED FLOW
          10       UF PERMEATE FLOW
```

Figure 5.8. Output corresponding to the data in Figure 5.7.

5.4 Configuration (*C)

The plant configuration is specified by the information contained in the input data deck.

For each unit in the plant, two data cards are entered. The first card specifies the unit number, equipment type, stream connections, and the descriptor for that item of equipment. The second card specifies the physical parameters for the respective item of equipment*

Table 5.2 gives the format for the first card. The format for the second card is always 8F10.0. The significance of the streams depends upon the equipment type, and is summarized in Table 5.3. Table 5.4 summarizes the data input specifications for the basic equipment types provided by the simulator. Note: The second card is always required, even though no parameters are to be read for that respective piece of equipment.

In the stream specifications, a positive stream number designates an input stream; a negative stream number designates an output stream.

To illustrate, suppose the following specifications are given for a unit of equipment:

```
3        OT        1        2        -3        BAD ACTOR WASTE TANK
500.        1700.        50.        50.    756.
```

The output listing generated in the configuration section is shown in Figure 5.9. Observe that descriptors accompany the stream numbers, and that engineering units accompany the parameters in the output listing.

For the plant whose flow sheet is given in Figure 5.10, Figure 5.11 lists the configuration data segment. Figure 5.12 provides the output for this configuration.

---

* some pieces of equipment require two parameter cards, refer to the specific sections in Chapter 3.

Table 5.2

Configuration Data Card #1

Quantity	Columns	Format
Equipment Number	2-5	I4
Equipment Type	9-10	A2
Stream #1	11-15	I5
Stream #2	16-20	I5
Stream #3	21-25	I5
Stream #4	26-30	I5
Stream #5	31-35	I5
Descriptor	41-60	5A4

Table 5.3

Significance of Streams

Equipment Type	Equipment Mnemonic	Stream #1	Stream #2	Stream #3	Stream #4	Stream #5
Mixed Tank	MT	I or 0	I or 0	I or 0	I or 0	I or 0
Overflow Tank	OT	Overflow Stream (0)	I or 0	I or 0	I or 0	I or 0
Pump	P	I	0	U	U	U
Stream Splitter	SP	I	Fixed Flow (0)	0	U	U
Stream Source	SO	0 Output	U	U	U	U
Stream Mixer	SM	Output stream must be specified last				U
Sink	SK	I	I	I	I	I
Ultrafiltration	UF	Permeate (0)	Concentrate (0)	Feed (I)		U
Gel model UF	GM	Permeate (0)	Concentrate (0)	Feed (I)	U	U
Reverse Osmosis	RO	Permeate (0)	Concentrate (0)	Feed (I)	U	U
Tubular RO	TR	Permeate (0)	Concentrate (0)	Feed (I)	U	U
UV/Ozonation	UV	I	0	U	U	U
Hypochlorination	HC	I	0	U	U	U

I = Input, 0 = Output, U = Unused

Table 5.4

Definition of Equipment Parameters

Equipment	Parameter	Quantity
MT	1	Initial volume in tank, m^3
	2	Initial suspended solids concentration, g/m^3
	3	Initial dissolved solids concentration, g/m^3
	4	Initial TOC concentration, g/m^3
OT	1	Initial volume in tank, m^3
	2	Initial suspended solids concentration, g/m^3
	3	Initial dissolved solids concentration, g/m^3
	4	Initial TOC concentration, g/m^3
	5	Design overflow, m^3/hr
	6	Maximum volume, m^3
P	1	Pump flow, m^3/hr
SP	1	Flow rate of fixed stream, m^3/hr
SO	1	Time of first pulse, hr
	2	Time duration of pulse, hr
	3	Time of cycle, hr
	4	Flow rate during pulse, m^3hr
	5	Suspended Solids concentration, g/m^3
	6	Dissolved solids concentration, g/m^3
	7	TOC concentration, g/m^3
SM	None	
SK	None	
UF, TR, GM	1	Number of Tubes
	2	Temperature °K
	3	Pressure drop across membrane at inlet
	4	Pressure drop down tube, atm
	5	Tube diameter, m
	6	Tube Length, m
RO	1	Pressure drop across the membrane, atm
	2	Temperature of feed, °K
	3	Length of fibers, m
	4	Outer radius of fiber bundle, m
	5	Inner radius of fiber bundle, m
	6	Fiber diameter, m

Table 5.4
(continued)

Equipment	Parameter	Quantity
RO	6	Fiber diameter 3, m
UV	1	Initial suspended solids concentration, g/m^3
	2	Initial dissolved solids concentration, g/m^3
	3	Initial TOC concentration, g/m^3
	4	Inlet gas phase ozone to air mass ratio
	5	Volumetric gas flow rate, m^3/hr
	6	Precontactor
	7	Number fo stages
	8	Contactor area, m^2
	9	Pre-contactor area, m^2
	10	Stage height, m
	11	Feed temperature, °K
	12	Operating Pressure, atm
HC	1	pH of the output
	2	Initial $Na(O\ Cl)_2$ in the HC unit
	3	Initial suspended solids concentration, g/m^3
	4	Initial dissolved solids concentration, g/m^3
	5	Initial TOC concentration, g/m^3
	6	Feed rate of $Ca\ (O\ Cl)_2$, m^3/hr
	7	Volume, m^3
	8	$Ca\ (O\ Cl)_2$ feed concentration, g/m^3

```
UNIT NO.    3            OVERFLOW TANK        BAD ACTOR WASTE TANK
     INPUT  STREAMS
              1     LABORATORY WASTE
              2     X-RAY WASTE
     OUTPUT STREAMS
              3     BAD ACTOR FLOW
     INITIAL CONDITIONS
          VOLUME OF TANK           .50000     CU.M
          SUSPENDED SOLIDS         160.00     G/M3
          DISSOLVED SOLIDS         1700.0     G/M3
          TOTAL ORG CARBON         263.73     G/M3
     DESIGN PARAMETERS
          DESIGN OVERFLOW RATE     .50000E-01 M3/H
          MAXIMUM VOLUME           .75600     CU.M
```

Figure 5.9. Example of the output generated in the configuration section.

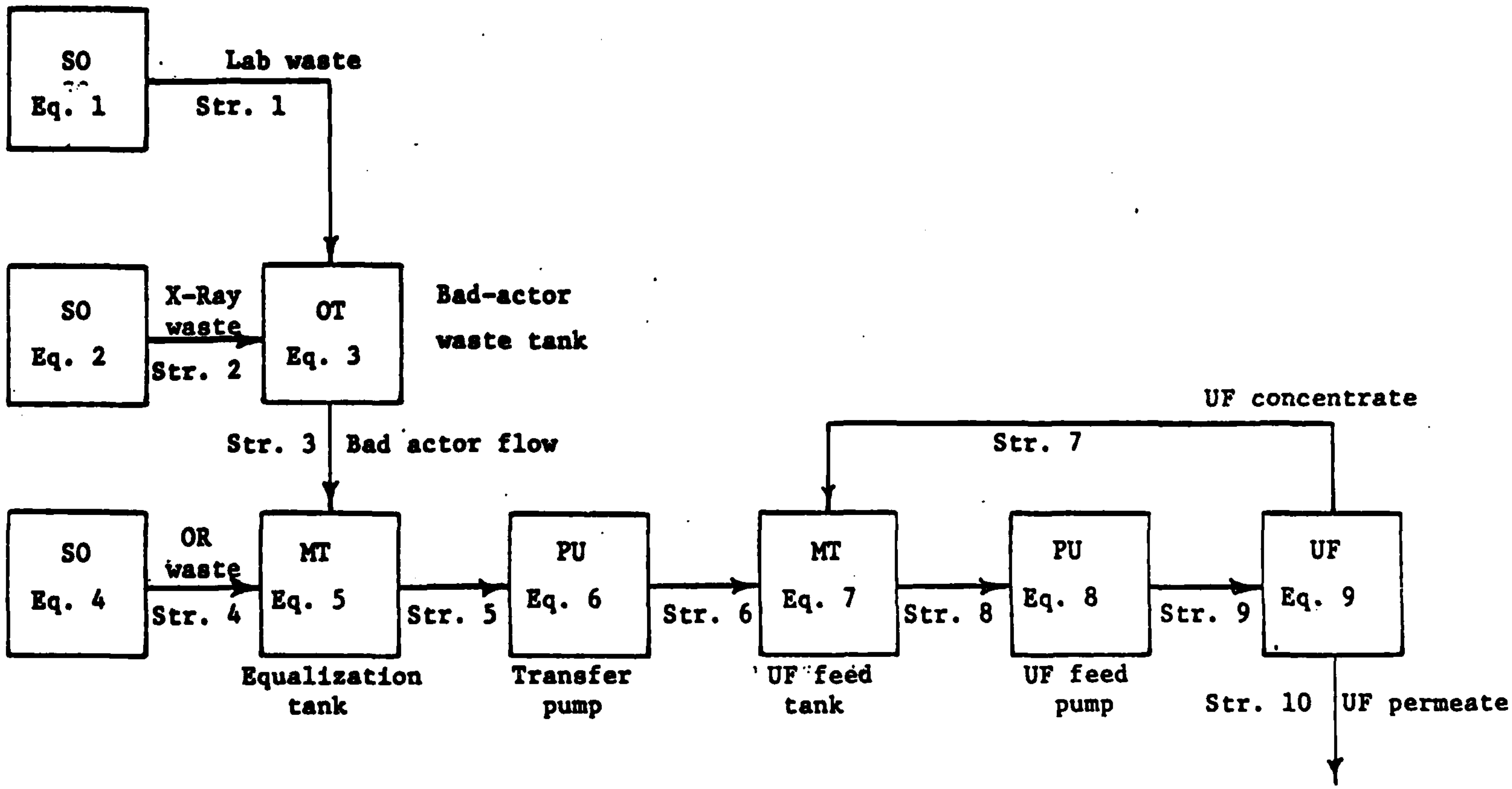


Figure 5.10. Simplified flowsheet for the equalization/prescreening and ultrafiltration sections of the WPE.

```
*C
     1    SO    -1                                  LAB WASTE SOURCE
9.         7.          24.          .189            58.8        2151.
     2    SO    -2                                  X-RAY WASTE SOURCE
9.         8.          24.          .06615          43.         1247.
     3    OT    -3                                  BAD ACTOR WASTE TANK
.5         160.        1700.        263.73         .05         .756
     4    SO    -4                                  O. R. WASTE SOURCE
0.         .25         .75          .5292           2.          1788.
     5    MT     3     4   -5                       EQUALIZATION TANK
2.5        160.        1700.        263.73
     6    P      5    -6                            EQ TANK PUMP
.270
     7    MT     6     7   -8                       UF FEED TANK
.5         160.        1700.        263.73
     8    P      8    -9                            UF FEED PUMP
2.
     9    UF   -10    -7    9                       UF MODULE
4.         311.1       3.4          2.04            .0254       20.49
 9999     SK    10

*
```

Figure 5.11. Configuration data segment for the plant in Figure 5.10.

```
*C        PLANT CONFIGURATION

UNIT NO.     1          STREAM SOURCE        LAB WASTE SOURCE
     INPUT  STREAMS
          NONE
     OUTPUT STREAMS
              1     LABORATORY WASTE
     INITIAL CONDITIONS
          NONE
     DESIGN PARAMETERS
          TIME OF FIRST PULSE      9.0000       HR
          PULSE DURATION           7.0000       HR
          PULSE CYCLE TIME         24.000       HR
          PULSE FLOW RATE          .18900       M3/H
          SUSPENDED SOLIDS         58.800       G/M3
          DISSOLVED SOLIDS         2151.0       G/M3
          TOTAL ORG CARBON         476.00       G/M3

UNIT NO.     2          STREAM SOURCE        X-RAY WASTE SOURCE
     INPUT  STREAMS
          NONE
     OUTPUT STREAMS
              2     X-RAY WASTE
     INITIAL CONDITIONS
          NONE
     DESIGN PARAMETERS
          TIME OF FIRST PULSE      9.0000       HR
          PULSE DURATION           8.0000       HR
          PULSE CYCLE TIME         24.000       HR
          PULSE FLOW RATE          .66150E-01   M3/H
          SUSPENDED SOLIDS         43.000       G/M3
          DISSOLVED SOLIDS         1247.0       G/M3
          TOTAL ORG CARBON         126.00       G/M3

UNIT NO.     3          OVERFLOW TANK        BAD ACTOR WASTE TANK
     INPUT  STREAMS
              1     LABORATORY WASTE
              2     X-RAY WASTE
     OUTPUT STREAMS
              3     BAD ACTOR FLOW
     INITIAL CONDITIONS
          VOLUME OF TANK           .50000       CU.M
          SUSPENDED SOLIDS         160.00       G/M3
          DISSOLVED SOLIDS         1700.0       G/M3
          TOTAL ORG CARBON         263.73       G/M3
     DESIGN PARAMETERS
          DESIGN OVERFLOW RATE     .50000E-01   M3/H
          MAXIMUM VOLUME           .75600       CU.M
```

Figure 5.12. Configuration output for the data in Figure 5.11.

```
UNIT NO.     4          STREAM SOURCE        O. R. WASTE SOURCE
     INPUT  STREAMS
          NONE
     OUTPUT STREAMS
              4      OPERATING ROOM WASTE
     INITIAL CONDITIONS
          NONE
     DESIGN PARAMETERS
          TIME OF FIRST PULSE         .0          HR
          PULSE DURATION              .25000      HR
          PULSE CYCLE TIME            .75000      HR
          PULSE FLOW RATE             .52920      M3/H
          SUSPENDED SOLIDS            2.0000      G/M3
          DISSOLVED SOLIDS            1788.0      G/M3
          TOTAL ORG CARBON            252.00      G/M3

UNIT NO.     5          MIXED TANK           EQUALIZATION TANK
     INPUT  STREAMS
              3      BAD ACTOR FLOW
              4      OPERATING ROOM WASTE
     OUTPUT STREAMS
              5      EQUILIZATION TK DISC
     INITIAL CONDITIONS
          VOLUME OF TANK              2.5000      CU.M
          SUSPENDED SOLIDS            160.00      G/M3
          DISSOLVED SOLIDS            1700.0      G/M3
          TOTAL ORG CARBON            263.73      G/M3
     DESIGN PARAMETERS
          NONE

UNIT NO.     6          PUMP                 EQ TANK PUMP
     INPUT  STREAMS
              5      EQUILIZATION TK DISC
     OUTPUT STREAMS
              6      EQ TK PUMP DISCHARGE
     INITIAL CONDITIONS
          NONE
     DESIGN PARAMETERS
          PUMP FLOW RATE              .27000      M3/H

UNIT NO.     7          MIXED TANK           UF FEED TANK
     INPUT  STREAMS
              6      EQ TK PUMP DISCHARGE
              7      RECYCLE FROM UF
     OUTPUT STREAMS
              8      UF FEED PUMP SUCTION
     INITIAL CONDITIONS
          VOLUME OF TANK              2.5000      CU.M
          SUSPENDED SOLIDS            160.00      G/M3
          DISSOLVED SOLIDS            1700.0      G/M3
          TOTAL ORG CARBON            263.73      G/M3
     DESIGN PARAMETERS
          NONE
```

Figure 5.12. (continued)

```
UNIT NO.     8           PUMP                    UF FEED PUMP
     INPUT  STREAMS
             8     UF FEED PUMP SUCTION
     OUTPUT STREAMS
             9     UF MODULE FEED FLOW
     INITIAL CONDITIONS
          NONE
     DESIGN PARAMETERS
          PUMP FLOW RATE              2.0000     M3/H


UNIT NO.     9           ULTRAFILTRATION         UF MODULE
     INPUT  STREAMS
             9     UF MODULE FEED FLOW
     OUTPUT STREAMS
            10     UF PERMEATE FLOW
             7     RECYCLE FROM UF
     INITIAL CONDITIONS
          NONE
     DESIGN PARAMETERS
          NUMBER OF TUBES             4.0000
          FEED TEMPERATURE            311.10     DEGK
          INLET DELTA P               3.4000     ATM
          DELTA P DOWN TUBE           1.3600     ATM
          TUBE DIAMETER               .25400E-01 M
          TUBE LENGTH                 20.490     M

UNIT NO. 9999            STREAM SINK
     INPUT  STREAMS
            10     UF PERMEATE FLOW
     OUTPUT STREAMS
          NONE
     INITIAL CONDITIONS
          NONE
     DESIGN PARAMETERS
          NONE
```

Figure 5.12. (continued)

Upon completion of the entry of the plant configuration, a check is made to see that for each stream

a) one and only one source is specified, and

b) one and only one destination is specified.

When a duplicate source definition or a duplicate destination definition is encountered, messages are generated in the configuration output. Figure 5.13 gives the stream summary printed after all units have been specified.

If any errors are detected in either the configuration or in the parameters specified, the run is terminated. The errors in the configuration section should be corrected and the run repeated.

STREAM SUMMARY

STREAM	SOURCE	DESTINATION
1	1	3
2	2	3
3	3	5
4	4	5
5	5	6
6	6	7
7	9	7
8	7	8
9	8	9
10	9	9999

Figure 5.13. Stream summary generated for the data in Figure 5.11.

5.5 Print Specifications (*PR)

The simulator will generate a tabular listing of up to ten process variables as a function of time. The output may be specified to be either of the following:

1. Any element of any stream, or
2. Any parameter associated with any unit of equipment.

At least one print specification must be made if an off-line storage specification is not made (See Section 5.6).

The specifications are entered, one per data card, as follows:

Col. 2-5: stream number or unit number, with the latter being entered as a negative number,

Col. 6-10: element number or parameter number.

Figure 5.14 lists a typical print specification segment of the input data deck. Figure 5.15 gives the output of the specification data. Observe that descriptors accompany all stream numbers, element numbers, equipment numbers, and parameter numbers. Figure 5.16 gives the tabular output generated during the execution of the simulation.

```
*PR
.4
     9     2
     9     3
    10     1
    10     2
    10     3
    -7     1
     5     2
     5     2
    -5     1
*
```

Figure 5.14. Typical print specification segment of the input data deck.

```
*PR       PRINT SPECIFICATIONS

     PRINT INTERVAL IS    .40000     HRS

-----STREAM       9      UF MODULE FEED FLOW
     ELEMENT      2      SUSPENDED SOLIDS
-----STREAM       9      UF MODULE FEED FLOW
     ELEMENT      3      DISSOLVED SOLIDS
-----STREAM       9      UF MODULE FEED FLOW
     ELEMENT      4      TOT. ORG CARBON
-----STREAM      10      UF PERMEATE FLOW
     ELEMENT      1      FLOW RATE
-----STREAM      10      UF PERMEATE FLOW
     ELEMENT      2      SUSPENDED SOLIDS
-----STREAM      10      UF PERMEATE FLOW
     ELEMENT      3      DISSOLVED SOLIDS
+++++UNIT         7      UF FEED TANK
     PARAMETER    1       VOLUME OF TANK
-----STREAM       5      EQUILIZATION TK DISC
     ELEMENT      2      SUSPENDED SOLIDS
-----STREAM       5      EQUILIZATION TK DISC
     ELEMENT      3      DISSOLVED SOLIDS
+++++UNIT         5      EQUALIZATION TANK
     PARAMETER    1       VOLUME OF TANK
```

Figure 5.15. Output of the print specification data.

TIME	STRM 9 ELE. 2	STRM 9 ELE. 3	STRM 9 ELE. 4	STRM 10 ELE. 1	STRM 10 ELE. 2
.0	160.	.170E+04	264.	1.27	.0
.400	194.	.170E+04	294.	1.06	.0
.800	232.	.170E+04	332.	.902	.0
1.20	275.	.170E+04	376.	.788	.0
1.60	321.	.170E+04	426.	.700	.0
2.00	372.	.171E+04	481.	.629	.0
2.40	427.	.171E+04	542.	.572	.0
2.80	486.	.171E+04	606.	.524	.0
3.20	549.	.171E+04	675.	.483	.0
3.60	613.	.171E+04	745.	.448	.0
4.00	679.	.171E+04	816.	.418	.0
4.40	745.	.171E+04	887.	.392	.0
4.80	809.	.171E+04	955.	.369	.0
5.20	869.	.172E+04	.102E+04	.348	.0
5.60	925.	.172E+04	.108E+04	.330	.0
6.00	974.	.172E+04	.112E+04	.313	.0
6.40	.101E+04	.172E+04	.117E+04	.298	.0
6.80	.105E+04	.172E+04	.120E+04	.285	.0
7.20	.107E+04	.172E+04	.122E+04	.272	.0
7.60	.109E+04	.173E+04	.123E+04	.261	.0
8.00	.109E+04	.173E+04	.123E+04	.251	.0
8.40	.109E+04	.173E+04	.123E+04	.241	.0
8.80	.108E+04	.173E+04	.122E+04	.232	.0
9.20	.107E+04	.173E+04	.121E+04	.224	.0
9.60	.105E+04	.173E+04	.119E+04	.216	.0
10.0	.103E+04	.174E+04	.116E+04	.209	.0
10.4	.100E+04	.174E+04	.114E+04	.202	.0
10.8	972.	.174E+04	.111E+04	.196	.0
11.2	943.	.174E+04	.109E+04	.190	.0
11.6	914.	.174E+04	.106E+04	.184	.0
12.0	884.	.175E+04	.103E+04	.179	.0
12.4	854.	.175E+04	.100E+04	.174	.0
12.8	824.	.175E+04	978.	.169	.0
13.2	796.	.175E+04	954.	.165	.0
13.6	768.	.176E+04	930.	.161	.0
14.0	741.	.176E+04	909.	.156	.0
14.4	715.	.176E+04	888.	.153	.0
14.8	691.	.177E+04	869.	.149	.0
15.2	667.	.177E+04	851.	.146	.0
15.6	644.	.178E+04	833.	.142	.0
16.0	623.	.178E+04	817.	.139	.0
16.4	602.	.178E+04	801.	.136	.0
16.8	582.	.178E+04	786.	.133	.0
17.2	563.	.179E+04	771.	.130	.0
17.6	545.	.179E+04	757.	.128	.0
18.0	528.	.179E+04	744.	.125	.0
18.4	512.	.179E+04	731.	.123	.0
18.8	496.	.179E+04	719.	.120	.0
19.2	482.	.179E+04	707.	.118	.0
19.6	467.	.180E+04	696.	.116	.0
20.0	454.	.180E+04	685.	.114	.0

Figure 5.16. Tabular output generated during the simulation

STRM 10	UNIT 7	STRM 5	STRM 5	UNIT 5
ELE. 3	PAR. 1	ELE. 2	ELE. 3	PAR. 1
.170E+04	2.50	160.	.170E+04	2.50
.170E+04	2.15	152.	.170E+04	2.54
.170E+04	1.86	150.	.170E+04	2.48
.170E+04	1.63	144.	.171E+04	2.50
.170E+04	1.44	141.	.171E+04	2.46
.170E+04	1.28	137.	.171E+04	2.45
.170E+04	1.15	133.	.171E+04	2.44
.171E+04	1.04	130.	.171E+04	2.41
.171E+04	.947	125.	.171E+04	2.43
.171E+04	.869	124.	.171E+04	2.36
.171E+04	.804	117.	.172E+04	2.41
.171E+04	.750	118.	.172E+04	2.32
.171E+04	.706	112.	.172E+04	2.36
.171E+04	.670	112.	.172E+04	2.27
.171E+04	.643	106.	.173E+04	2.32
.172E+04	.622	107.	.173E+04	2.23
.172E+04	.608	101.	.173E+04	2.27
.172E+04	.599	101.	.173E+04	2.21
.172E+04	.595	96.7	.173E+04	2.23
.172E+04	.597	95.0	.173E+04	2.19
.172E+04	.602	92.4	.174E+04	2.18
.173E+04	.612	89.7	.174E+04	2.17
.173E+04	.625	88.3	.174E+04	2.14
.173E+04	.642	84.6	.174E+04	2.16
.173E+04	.662	83.7	.174E+04	2.09
.173E+04	.685	78.6	.175E+04	2.14
.173E+04	.711	78.5	.175E+04	2.05
.174E+04	.740	73.6	.175E+04	2.09
.174E+04	.771	73.5	.176E+04	2.00
.174E+04	.804	68.9	.176E+04	2.05
.174E+04	.839	68.8	.176E+04	1.96
.174E+04	.877	64.5	.176E+04	2.00
.175E+04	.916	63.4	.177E+04	2.01
.175E+04	.957	60.2	.178E+04	2.11
.175E+04	1.00	58.6	.179E+04	2.16
.176E+04	1.04	56.6	.179E+04	2.23
.176E+04	1.09	54.7	.180E+04	2.30
.177E+04	1.14	53.7	.180E+04	2.35
.177E+04	1.19	51.6	.180E+04	2.45
.177E+04	1.24	51.2	.181E+04	2.47
.178E+04	1.29	48.9	.181E+04	2.60
.178E+04	1.34	49.0	.181E+04	2.51
.178E+04	1.39	46.7	.181E+04	2.56
.178E+04	1.45	46.8	.181E+04	2.48
.179E+04	1.51	44.5	.181E+04	2.52
.179E+04	1.56	44.6	.181E+04	2.43
.179E+04	1.62	42.5	.180E+04	2.48
.179E+04	1.68	42.1	.180E+04	2.41
.179E+04	1.74	40.5	.180E+04	2.43
.179E+04	1.80	39.8	.180E+04	2.39
.179E+04	1.86	38.7	.180E+04	2.39

Figure 5.16. (continued)

5.6 Plot Specifications (*PL)

The simulator will generate plots of up to ten process variables as a function of time. The output may be specified to be either of the following:

1. Any element of any stream, or
2. Any parameter associated with any unit of equipment

If no plots are to be generated, the entire plot specification data segment should be omitted.

The first data card in the plot specification segment contains the time duration (in hours) for the plot in columns 1-10 (format is F10.0). The following cards contain the specifications entered one per card, as follows:

Col. 2-5: stream number or equipment number, with the latter being entered as a negative number

Col. 6-10: element number or parameter number

Figure 5.17 lists a typical plot specification segment of the input data deck. Figure 5.18 gives the output of the specification data. The plots themselves will be presented in a later section.

The plots are not generated as the simulation is being executed, but instead the values are stored in arrays for plotting upon completion of the run.

```
*PL
20.
   -5    1
    9    2
    9    3
   10    1
   -7    1
*
```

Figure 5.17. Typical plot specification segment of the input data deck.

```
*PL       PLOT VARIABLES

     PLOT DURATION   20.00 HRS

+++++UNIT          5     EQUALIZATION TANK
     PARAMETER     1      VOLUME OF TANK
-----STREAM        9     UF MODULE FEED FLOW
     ELEMENT       2     SUSPENDED SOLIDS
-----STREAM        9     UF MODULE FEED FLOW
     ELEMENT       3     DISSOLVED SOLIDS
-----STREAM       10     UF PERMEATE FLOW
     ELEMENT       1     FLOW RATE
+++++UNIT          7     UF FEED TANK
     PARAMETER     1      VOLUME OF TANK
```

Figure 5.18. Output of the plot specification data.

5.7 Run Specifications (*RUN)

This section is used to specify to the simulator the total run time and the integration step size to use. These values are entered on a single card with FORMAT (2F10.0). Figure 5.19 lists a typical run specification segment of the data deck. Figure 5.20 gives the output generated by the *RUN section.

```
*RUN
20.        .001
*
```

Figure 5.19. Typical run control data.

```
*RUN       RUN TIME PARAMETERS
     TOTAL TIME FOR RUN   20.00      HRS
     INTEGRATION STEP SIZE   .1000E-02 HRS
```

Figure 5.20. Output from run control section.

Upon completion of the simulation, the simulator prints a material balance showing

1. Initial inventory
2. Amount input (from sources)
3. Final inventory
4. Amount output (to sink)

A typical material balance output is given in Figure 5.19. Due to round-off errors, the material balance does not generally close exactly (except for plants with small configurations). However, large errors would indicate a problem somewhere in the coding.

*****MATERIAL BALANCE*****

	INITIAL INVENTORY	AMOUNT INPUT	TOTAL IN
VOLUME	5.50	5.42	10.9
SUSPENDED SOLIDS	880.	108.	988.
DISSOLVED SOLIDS	.935E+04	.990E+04	.192E+05
TOTAL ORGANIC CARBON	.145E+04	.160E+04	.305E+04

FINAL INVENTORY	AMOUNT OUTPUT	TOTAL OUT	DIFFERENCE
4.85	6.02	10.9	.480E-01
971.	.0	971.	16.4
.877E+04	.104E+05	.191E+05	132.
.218E+04	832.	.302E+04	31.7

Figure 5.19. Simulator Output of Material Balance Calculations.

5.8 Plot Control (*PC)

As indicated in an earlier section, a maximum of ten variables can be plotted. The simulator permits the output to be one plot containing all ten variables, to be ten plots containing one variable each, or to be any combination thereof.

For each variable to be plotted, a data card must be entered containing the following information:

Quantity	Columns	Format
Plot Character	1	A1
Zero-coordinate	6-15	F10.0
Maximum-coordinate	16-25	F10.0

The plot grid is 40 rows by 100 columns.

The existence of a blank card in the data deck indicates to the simulator that a plot is to be generated containing the variables for which the plot parameters have been given. To illustrate, a typical plot control data segment is illustrated in Figure 5-22. A total of four plots will be generated. For all plots except the second, a single variable will be plotted. One the second plot, two variables will be plotted. When more than one variable is to be plotted, the y-coordinates are always that of the first variable for that respective plot. Figure 5-23 illustrate the second plot generated from the data in Figure 5-22.

```
*PC
L     2000.     2800.

S     5.        25.
D     2000.     10000.

P     0.        400.

L     200.      1400.

*
```

Figure 5.22. Typical plot control segment of the input data deck.

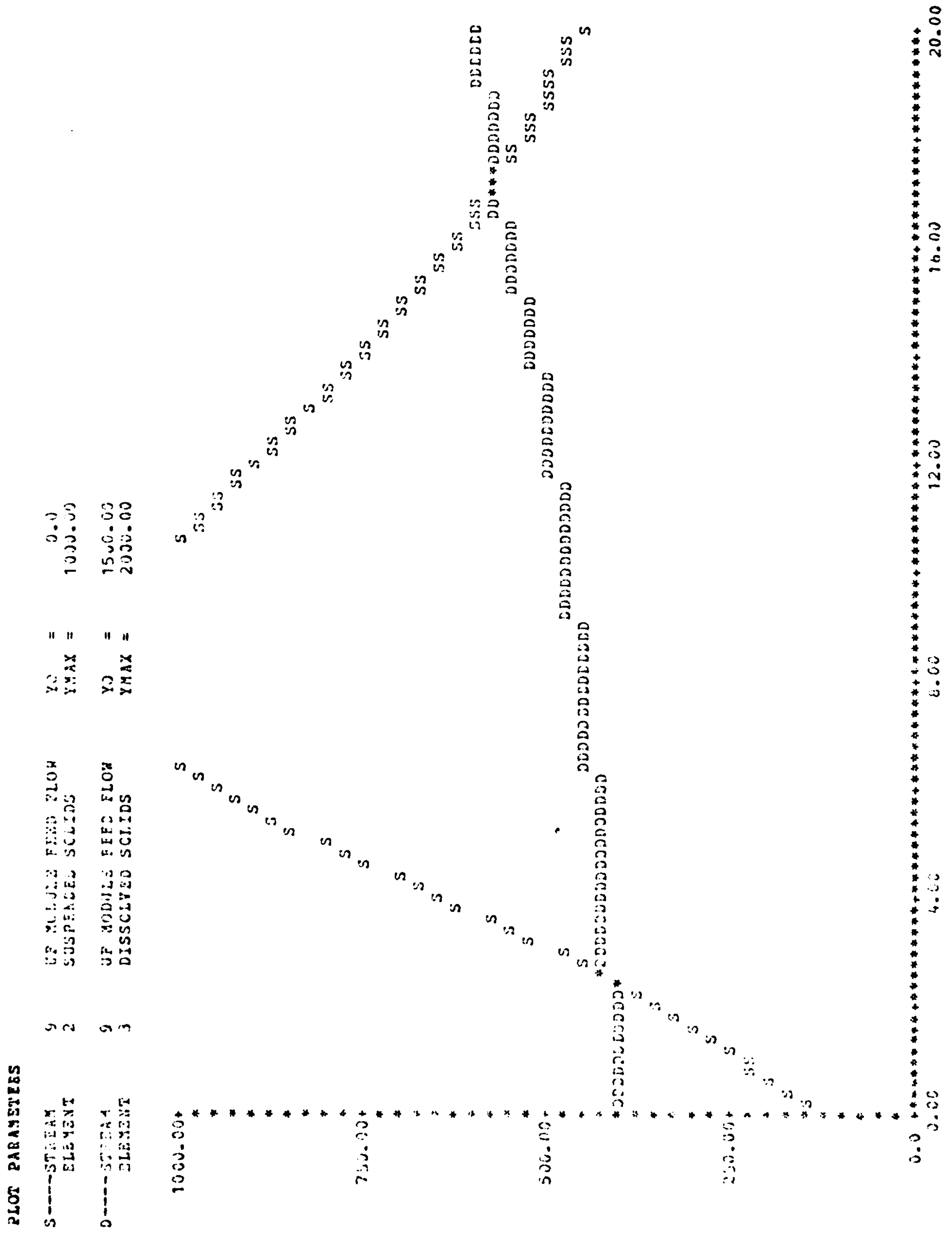


Figure 5.23. Second plot generated from the data in Figure 5.19.

5.9 Off-line Storage (*OF)

This section allows for the storage of the values of up to 50 process variables, which may be retrieved for printing and/or plotting at a latter date (see section 5.11). The values are written to FORTRAN logical unit number 8, which should be connected to a sequential dataset with a logical record length of one byte.

The first data card must be a unique message that uniquely identifies the particular run. The next data card is a flag that tells the simulator where on the dataset to store the values of the run. There are two choices; FORMAT (I2):

1) -1 tells the simulator to start at the very beginning of the dataset (this is required if the dataset has never been used by the simulator)
2) +1 tells the simulator to start at the end of the last set of values on the dataset (in valid for a new dataset)

The third card is the save interval, i.e., the time interval between saves.

After the third card, the process variables to be saved are specified, one per card, just as in the print segment. See section 5.5 for what variables may be saved, and the format of each data card. Figure 5.24 lists a typical off-line specification segment of the input data deck. Figure 5.25 gives the output fo the off-line segment.

Note that this segment must be specified after the configuration section, and before the run section.

```
*OF
-1
RUN NUMBER ABC123
.4
    9     2
    9     3
    9     4
   10     1
   10     2
   10     3
   -7     1
    5     2
    5     3
   -5     1
*
```

Figure 5.24. Sample input data for Off-line Storage

```
*OF       OFF-LINE PARAMETER LIST
THE HEADER MESSAGE FOR THE DATA SET IS
RUN NUMBER ABC123
THE DATA SET WILL BE CLEARED, AND THE NEW VALUES SAVED FROM THE BEGINNING.
THE SAVE INTERVAL IS    .4000
-----STREAM       9      UF MODULE FEED FLOW
     ELEMENT      2      SUSPENDED SOLIDS
-----STREAM       9      UF MODULE FEED FLOW
     ELEMENT      3      DISSOLVED SOLIDS
-----STREAM       9      UF MODULE FEED FLOW
     ELEMENT      4      TOT. ORG CARBON
-----STREAM      10      UF PERMEATE FLOW
     ELEMENT      1      FLOW RATE
-----STREAM      10      UF PERMEATE FLOW
     ELEMENT      2      SUSPENDED SCLIDS
-----STREAM      10      UF PERMEATE FLOW
     ELEMENT      3      DISSCLVED SOLIDS
+++++UNIT         7      UF FEED TANK
     PARAMETER    1       VOLUME OF TANK
-----STREAM       5      EQUILIZATION TK DISC
     ELEMENT      2      SUSPENDED SCLIDS
-----STREAM       5      EQUILIZATION TK DISC
     ELEMENT      3      DISSOLVED SCLIDS
+++++UNIT         5      EQUALIZATION TANK
     PARAMETER    1       VCLUME OF TANK
```

Figure 5.25. Simulator output for the data given in Figure 5.24.

5.10 Old Value Retrieval (*OL)

This segment indicates to the simulator that no simulation is to be performed, rather, values are to be read from a dataset on which values of a previous run have been stored by use of the off-line storage feature (see section 5.10). The dataset must be connected to FORTRAN logical unit number 8.

The only card in this section must contain the identification message of the data to be retrieved. This message must be identical to the message used in the off-line storage run. Figure 5.26 gives the corresponding *OL message for the *OF message of Figure 5.24. Figure 5.27 gives the corresponding output.

Note that *OL and *RUN are mutually exclusive. Also, the *SE, *SN, and *C sections must be specified again, exactly as in the original simulation run.

```
*OL
RUN NUMBER ABC123
*
```

Figure 5.26. Sample data to retrieve the values saved by the data in Figure 5.24.

```
*OL            OLD VALUES SPECIFICATIONS
RUN NUMBER ABC123
```

Figure 5.27. Simulator output for the *OL data given in Figure 5.26.

LISTING OF

SOURCE PROGRAM

```
      SUBROUTINE WPE
C   WPE  SIMULATOR
C
C   THIS IS THE MAIN ROUTINE FOR THE SIMULATION PACKAGE
C
      COMMON /LOOK/   ISW
      COMMON /MATDIS/ MATCAL
      COMMON STREAM(4,100), ICONFG(8,100), PAR(500), NPAR,
     &        NCALL, IUNIT, NFATER, NS, NEQ, DESC(5)
      COMMON /CTIME/  TIME, FTIME, DT
      COMMON /CPLOT/  NPLOT, TPLOT, KPLOT, PLTDTA(100,10),
     &                JPSTRM(2,10)
      COMMON /CPRINT/ IPRINT, NPELE, KPRINT(2,10)
      COMMON /COFLN/  NPL, LIST(2,50), LABLE, TOFLN,
     &                MESSAG(20), IEOF, IHEAD
      COMMON /MATBAL/ BALNCE(4), AMTIN(4), AMTOUT(4)
      DIMENSION BALNC(4), TOTIN(4), TOTOUT(4), DIFF(4)
C   NPAR - NUMBER OF PARAMETERS FOR UNIT I
C          (INDEX INTO ARRAY PAR)
C   NCALL - SUBROUTINE CALCULATION SELECTION
C      -1 - READ PARAMETERS
C       0 - INITIALIZATION
C       1 - SIMULATE
C   NPELE - NUMBER OF PRINT ELEMENTS
C   NPLOT - NUMBER OF PLOT ELEMENTS
C   NOFLIN- NUMBER OF OFF-LINE ELEMENTS
C   KPLOT - INDEX (2) INTO     ARRAY PLTDTA
C   STREAM(4,100) - STREAM VECTORS (FLOW,SS,TDS,TOC)
C   ICONFG(8,100) - CONFIGURATION ARRAY
C    (UNIT#,TYPE CODE,STRM1,...,STRM5,NPAR)
C   PAR(500) - PARAMETER VECTOR
C   KPRINT -  STREAM/ELEMENT DESIGNATION OF PRINT OUTPUTS
C   JSCK(2,100) - STREAM CHECK ARRAY
C   JPSTRM(2,10) - STREAM/ELEMENT DESIGNATION OF PLOT OUTPUTS
C   PLTCRD(2,10) - YO/YMAX FOR PLOT OUTPUTS
C   PLTDTA(100,10) - PLOT DATA
      CALL ERRSET(208,0,-1,1)
      DO 10 J=1,100
      DO 10 I=1,4
   10 STREAM(I,J)= 0.0
      ISW= 0
      NFATER= 0
C   READ CONFIGURATION AND PARAMETERS
      CALL RDATA
        TIME= -DT
      DTPLOT= .01*TPLOT
      XPRINT= 0.0
       XOFLN= 0.0
       XPLOT= 0.0
      IF(NPL .LT. 0.) GO TO 60
C   GET INITIAL INVENTORY
      MATCAL= 0
       NCALL= -2
```

```
      DO 20 IUNIT= 1, NEQ
        NPAR= ICONFG(8,IUNIT)
   20 CALL SUBCAL
      DO 30 I=1,4
       BALNO(I) = BALNCE(I)
   30 BALNCE(I) = 0.
C  PERFORM INITIALIZATION CALCULATIONS
       NCALL= 0
   40 IF(NPL .LT. 0.) GO TO 60
      DO 50 IUNIT=1,NEQ
        NPAR= ICONFG(8,IUNIT)
   50 CALL SUBCAL
      IF(NFATER .GT. 10) STOP 45
C  PERFORM SIMULATION
       NCALL= 1
   60   TIME= TIME + DT
      DTIME= TIME + .01*DT
      IF(NPL .EQ. 0) GO TO 80
      IF(DTIME .LT. XOFLN) GO TO 80
       XOFLN= XOFLN + TOFLN
      IF(NPL .GT. 0) CALL SAVEIT
      IF(NPL .LT. 0) CALL GETIT
   80 IF(NPELE .EQ. 0) GO TO 90
      IF(DTIME .LT. XPRINT) GO TO 90
      XPRINT= XPRINT + TPRINT
      CALL PRINT
   90 IF(NPLOT .EQ. 0) GO TO 100
      IF(DTIME .LT. XPLOT) GO TO 100
      XPLOT= XPLOT + DTPLOT
      CALL PLOT2
  100 IF(DTIME .LT. FTIME) GO TO 40
      IF(NPL .LT. 0) GO TO 160
      IF(NPL .NE. 0) WRITE(8,110) IEOF
      IF(NPL .NE. 0) ENDFILE 8
  110 FORMAT(A4)
C GET FINAL INVENTORY
      MATCAL= 1
       NCALL= -2
      DO 120 IUNIT=1,NEQ
        NPAR= ICONFG(8,IUNIT)
  120 CALL SUBCAL
      WRITE(6,130)
  130 FORMAT('1*****MATERIAL BALANCE*****'/32X,'INITIAL',7X,
     & 'AMOUNT',6X,'TOTAL',6X,'FINAL',8X,'AMOUNT',6X,'TOTAL'
     & 31X,'INVENTORY',7X,'INPUT',8X,'IN',5X,'INVENTORY',6X,
     & 'OUTPUT',7X,'OUT',4X,'DIFFERENCE')
      DO 140 I=1,4
       TOTIN(I)= AMTIN(I)  + BALNO(I)
      TOTOUT(I)= AMTOUT(I)  + BALNCE(I)
  140   DIFF(I)= TOTIN(I)  - TOTOUT(I)
      WRITE(6,150)  (BALNO(I),AMTIN(I),TOTIN(I),BALNCE(I),
     & AMTOUT(I),TOTOUT(I),DIFF(I),I=1,4)
  150 FORMAT(6X,'VOLUME',T29,7G12.3/6X,'SUSPENDED SOLIDS',
     & T29,7G12.3/6X,'DISSOLVED SOLIDS',T29,7G12.3/6X,
```

```
      & 'TOTAL ORGANIC CARBON',T29,7G12.3)
C MAKE PLOTS, IF NECESSARY
  160 IF(NPLOT .EQ. 0) STOP
      CALL PLOT3
      RETURN
      END
```

```
      BLOCK DATA
      REAL*8 HC1
      COMMON /CTIME/  TIME, FTIME, DT
      COMMON /COFLN/  NPL, LIST(2,50), LABLE, TOFLN,
     &                MESSAG(20), IEOF, IHEAD
      COMMON /CPLOT/  NPLOT, TPLOT, KPLOT, PLTDTA(100,10),
     &                JPSTRM(2,10)
      COMMON /CPRINT/ TPRINT, NPELE, KPRINT(2,10)
      COMMCN /CREAD/  IFIRST, IAST, ICARD(20)
      COMMON /MATBAL/ BALNCE(4), AMTIN(4), AMTOUT(4)
      COMMON /NAMES/  IUNITS(12), NMSTRM(5,100),
     &                NMEQPT(5,100), NMELE(5,5), ISUNIT(5),
     &                NMPAR(6,75), IDNMPR(150)
      COMMON /UFPARM/ UF1(2), IUF1(3)
      COMMON /UFFIT/  UF2(6)
      CCMMCN /PARMUF/ UF3(5)
      COMMON /TRPARM/ TR1(2), ITR1(3)
      COMMCN /TRFIT/  TR2(10)
      COMMON /PARMTR/ TR3(5)
      COMMON /GMPARM/ GM1(2), IGM1(3)
      CCMMON /GMFIT/  GM2(11)
      COMMCN /PARMGM/ GM3(5)
      COMMON /CHECK/  JSCK(2,100)
      COMMON /UFSAV1/ UFSAVE
      COMMCN /PARMRO/ RO1(6),IRO1(2)
      COMMON /ROFIT/  RO2(10)
      COMMCN /RCPARM/ RO3(4),IRO3(3)
      COMMCN /PIDSAV/ PIDSV(2)
      COMMON /UVFIT/  UV1(10)
      COMMCN /UVPARM/ UV2(6), IUV
      COMMON /STGSAV/ UV5(50)
      COMMON /STAGES/ UV4(2)
      CCMMCN /GASLAW/ RGAS
      COMMON /HCPARM/ HC1(5), IHC1(2)
      COMMON /HCSAV2/ HC2(3)
      DIMENSION NMPR(6,11), NMUF(6,8), NMUV(6,7), NMRO(6,3),
     &          NMEXTR(6,1), NMHC(6,3), NMPID(6,7),
     &          NMSN(6,4), NMMN(6,5), NMBIN(6,3)
      EQUIVALENCE (NMPR,NMPAR(1,1)), (NMUF,NMPAR(1,12)),
     &            (NMUV,NMPAR(1,20)),(NMRO,NMPAR(1,27)),
     &            (NMEXTR,NMPAR(1,30)),(NMHC,NMPAR(1,31)),
     &            (NMPID,NMPAR(1,34)),(NMSN,NMPAR(1,41)),
     &            (NMMN,NMPAR(1,45)),(NMBIN,NMPAR(1,50))
C  DATA STATEMENTS FOR ULTRAFILTRATION
      DATA IUF1  /3*0/, ITR1/3*0/
      DATA UF2   /71251., .40141, .14674E-3, .10537, 1.1185,
C                  G1        G2       GINFC1       C2
     &            0.46156E-2/
C                      CINF
      DATA UF3   /0.,  .003274,1.E6,  0.,      0./
C                TEMP   VISC   DENB DPZERO   PDROP
C  DATA STATEMENTS FOR TUBULAR RO
      DATA TR2   /1.91E4, 0.57895, 1.44E4, 1.0391E-8,
```

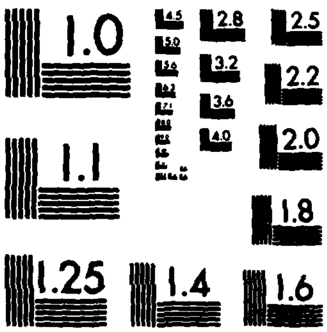
```
C                    GAM1     GAM2   GAMINF    API
     &             3.9526E-5, 4.2112E-3, 4.8E-2, 3.0254E-7,
C                       B          C         DCX       ADAX
     &             4.854E-06, 0.61405/, IGM1/3*0/
C                      BDAX      CDAX
      DATA TR3    /0., .003274, 1.E6,  0.,      0./
C                 TEMP  VISC    DENB DPZERO  PDROP
C  DATA STATEMENTS FOR GEL MODEL
      DATA GM2    /11*0.0/
      DATA GM3    /0., .003274, 1.E6,  0.,      0./
C                 TEMP  VISC    DENB DPZERO  PDROP
C  DATA STATEMENTS FOR FIBER REVERSE OSMOSIS
      DATA RO1    /0., 0., 0., 0., .05, .01/
C                  L    RO   RI   DP TOLMX TOLMN
      DATA IRO1  /0, 10/, IRO3/ 17,   22,    0/
C             NWRITE  NSTEPS  MCNT2 MCNT3  JWRITE
      DATA RO2/0.02117, 5.7434E-4, 3.791, 2.526E-7, 6.81E-5,
C                 AKA      AKC        ERE       API        BPI
     &             18.35, 2.488E-6, 1.351E-6, 3.694E7, .6295/
C                  GAMMA      B          C          NF     RATIO
      DATA RO3    /0.,  .003274, 0.,  1.E6/
C                TEMP    VISC   DELP  RHOB
C  DATA STATEMENTS FOR UV/OZONATION
      DATA UV1    /2.856E+6, 1.0, 4.125, 931.24, 0., 1.0,
C                  KHENRY   ECOZ  ETOC   KRATE KDCOMP EOZD
     &             0.,  1.6667E-4, 0.0, 16830./, IUV/0/
C                UVEFCT  RATIO      EN   QPRIME     NWRITE
      DATA UV2    / 0.,    0., 0., 55.556, 0.,   0./
C                 CAREA PAREA H   RHOB  PRESS  TEMP
      DATA RGAS  /.8205/
C  DATA STATEMENTS FOR HYPOCHLORINATION
      DATA HC1 /0.D0, 0.D0, 0.D0, .27D-7, 0.D0/
C                 VOL  ALPHA  RD     KEQ CAOCL2
      DATA HC2    /52500.0, 52500.0, 1.E6/, IHC1/0,   30/
C                  MWHOCL    MWOCL   RHO       JWRITE MCNT
      DATA NPL    /0/, TOFLN/0./, IEOF/'*EOF'/, IHEAD/'HEAD'/
      DATA NPLOT /0/, TPRINT/0./, NPELE/0/, IAST/'*'/
      DATA NMSTRM/500*'      '/, JSCK/200*0/, KPLOT/0/
      DATA BALNCE,AMTIN,AMTOUT/4*0.0, 4*0.0, 4*0.0/
      DATA IUNITS/'HR', 'M3/H', 'G/M3', 'CU.M', 'M', 'M2',
     &             'G/M3', 'M2/H', 'DEGK', 'ATM', ' ', ' '/
C  MT
      DATA IDNMPR/1,  4,  7,  5,  6, 30,
C  OT
     &             2,  6,  7,  5,  6, 30,  8,  9,
C  P
     &             3,  1, 10,
C  SP
     &             4,  1, 11,
C  SO
     &             5,  7,  1,  2,  3,  4,  5,  6, 30,
C  SM
     &             6,  0,
C  UF
```

```
     &              7,  6, 12, 13, 14, 15, 16, 17,
C  RO
     &              8,  6, 27, 13, 17, 28, 29, 18,
C  UV
     &              9, 12,  5,  6, 30, 20, 21, 22, 23, 24, 25,
     &                    26, 13, 27,
C  HC
     &             10,  8, 31, 32,  5,  6, 30, 33,  7, 19,
C  SK
     &             11,  0,
C  CN
     &             12,  7, 34, 35, 36, 37, 38, 39, 40,
C  SN
     &             13,  4, 41, 42, 43, 44,
C  MN
     &             14,  5, 45, 46, 47, 48, 49,
C  RC
     &             15,  5, 34, 35, 52, 40,
C  BC
     &             16,  8, 34, 35, 50, 51, 47, 48, 49, 40,
C  TR
     &             17,  6, 12, 13, 14, 15, 16, 17,
C  GM
     &             18,  6, 12, 13, 14, 15, 16, 17,
     &             23*0/
C  1
      DATA NMPR  /'TIME', ' OF ', 'FIRS', 'T PU', 'LSE ', 1,
     &            'PULS', 'E DU', 'RATI', 'ON  ', '    ', 1,
     &            'PULS', 'E CY', 'CLE ', 'TIME', '    ', 1,
     &            'PULS', 'E FL', 'OW R', 'ATE ', '    ', 2,
     &            'SUSP', 'ENDE', 'D SO', 'LIDS', '    ', 3,
     &            'DISS', 'OLVE', 'D SO', 'LIDS', '    ', 3,
     &            'VOLU', 'ME O', 'F TA', 'NK  ', '    ', 4,
     &            'DESI', 'GN O', 'VERF', 'LOW ', 'RATE', 2,
     &            'MAXI', 'MUM ', 'VOLU', 'ME  ', '    ', 4,
     &            'PUMP', ' FLO', 'W RA', 'TE  ', '    ', 2,
     &            'FIXE', 'D FL', 'OW R', 'ATE ', '    ', 2/
C 12
      DATA NMUF  /'NUMB', 'ER O', 'F TU', 'BES ', '    ',11,
     &            'FEED', ' TEM', 'PERA', 'TURE', '    ', 9,
     &            'INLE', 'T DE', 'LTA ', 'P   ', '    ',10,
     &            'DELT', 'A P ', 'DOWN', ' TUB', 'E   ',10,
     &            'TUBE', ' DIA', 'METE', 'R   ', '    ', 5,
     &            'TUBE', ' LEN', 'GTH ', '    ', '    ', 5,
     &            'FIBE', 'R DI', 'AMET', 'ER  ', '    ', 5,
     &            'CAOC', 'L2 F', 'EED ', 'CONC', '.   ', 3/
C 20
      DATA NMUV  /'GAS ', 'OZON', 'E CO', 'NC. ', '    ',11,
     &            'GAS ', 'FLOW', ' RAT', 'E   ', '    ', 2,
     &            'PREC', 'ONTA', 'CTOR', '    ', '    ',11,
     &            'NUMB', 'ER O', 'F ST', 'AGES', '    ',11,
     &            'CONT', 'ACTO', 'R AR', 'EA  ', '    ', 6,
     &            'PRE-', 'CONT', 'ACTO', 'R AR', 'EA  ', 6,
     &            'HEIG', 'HT O', 'F A ', 'STAG', 'E   ', 5/
```

```
C 27
      DATA NMRO   /'OPER', 'ATIN', 'G PR', 'ESSU', 'RE  ',10,
     &             'OUTE', 'R RA', 'DIUS', '    ', '    ', 5,
     &             'INNE', 'R RA', 'DIUS', '    ', '    ', 5/
C 30
      DATA NMEXTR/'TOTA', 'L OR', 'G CA', 'RBON', '    ', 7/
C 31
      DATA NMHC   /'PH  ', '    ', '    ', '    ', '    ',11,
     &             'FREE', ' CHL', 'ORIN', 'E   ', '    ',12,
     &             'CA(O', 'CL)2', '  FE', 'ED R', 'ATE ', 2/
C 34
      DATA NMPID /'SENS', 'OR I', 'D   ', '    ', '    ',11,
     &             'MANI', 'PULA', 'TOR ', 'ID  ', '    ',11,
     &             'SET ', 'POIN', 'T   ', '    ', '    ',11,
     &             'GAIN', '    ', '    ', '    ', '    ',11,
     &             'RESE', 'T TI', 'ME  ', '    ', '    ', 1,
     &             'RATE', ' TIM', 'E   ', '    ', '    ', 1,
     &             'MODE', '    ', '    ', '    ', '    ',11/
C 41
      DATA NMSN   /'UNIT', ' OR ', 'STRE', 'AM I', 'D   ',11,
     &             'ITEM', ' OF ', 'INQU', 'IRY ', '    ',11,
     &             'CURR', 'ENT ', 'READ', 'ING ', '    ',11,
     &             'TIME', ' CON', 'STAN', 'T   ', '    ', 1/
C 45
      DATA NMMN   /'UNIT', ' ID ', '    ', '    ', '    ',11,
     &             'MANI', 'PULA', 'TED ', 'ITEM', '    ',11,
     &             'CURR', 'END ', 'VALU', 'E   ', '    ',11,
     &             'UPPE', 'R LI', 'MIT ', '    ', '    ',11,
     &             'LOWE', 'R LI', 'MIT ', '    ', '    ',11/
C 50
      DATA NMBIN /'LOW ', 'SET ', 'POIN', 'T   ', '    ',11,
     &             'HI S', 'ET P', 'OINT', '    ', '    ',11,
     &             'RATI', 'O   ', '    ', '    ', '    ',11/
       END
```

AD-A143 024 MODELING AND SIMULATION OF WASTEWATER REUSE SYSTEMS - DYNAMIC PROCESS SIMULATOR(U) LOUISIANA STATE UNIV BATON ROUGE DEPT OF CHEMICAL ENGINEERING.. C L SMITH ET AL. 2/2

UNCLASSIFIED MAY 82 DAMD17-77-C-7040 F/G 9/2 NL



MICROCOPY RESOLUTION TEST CHART
NATIONAL BUREAU OF STANDARDS-1963-A

```
      SUBROUTINE RDATA
C
C THIS SUBROUTINE READS ALL INPUT DATA
C
      LOGICAL OFF/.FALSE./
      COMMON /CREAD/ IFIRST, IAST, ICARD(20)
      COMMON /CTIME/ TIME, FTIME, DT
      EQUIVALENCE (ICARD1,ICARD(1))
      DATA IMP, ISE, ISN, IC, IOF, IOL, IPR, IPL, IRUN/
     &     '*MP', '*SE', '*SN', '*C', '*OP', '*OL',
     &     '*PR', '*PL', '*RUN'/
C  READ FIRST CARD.  SHOULD BE A DATA CONTROL CARD
      CALL RCARD
C  FIRST CARD SHOULD BE *MP OR *SE
      IF(ICARD1 .EQ. IMP) GO TO 20
      IF(ICARD1 .EQ. ISE) GO TO 40
      WRITE(6,10) IMP, ISE, ICARD
   10 FORMAT('0*****EXPECTING ''',A4,''' OR ''',A4,
     & ''', FOUND '/' ''',20A4,'''')
      STOP
C  FOUND *MP, READ MODEL PARAMETERS
   20 CALL RMODPR
C  RETURN FROM RMODPR OCCURS ONLY WHEN A DATA CONTROL CARD
C  HAS BEEN ENCOUNTERED. THE NEXT CARD SHOULD BE *SE
      CALL RCARD
      IF(ICARD1 .EQ. ISE) GO TO 40
      WRITE(6,30) ISE, ICARD
   30 FORMAT('0*****EXPECTING ''',A4,''', FOUND'/
     &        ' ''',20A4,'''')
      STOP
C  FOUND *SE, READ STREAM ELEMENT DEFINITIONS
   40 CALL RSTRME
C  RETURN FROM RSTRME OCCURS ONLY WHEN A DATA CONTROL CARD
C  HAS BEEN ENCOUNTERED.  THE NEXT CARD SHOULD BE *SN OR *C
      CALL RCARD
      IF(ICARD1 .EQ. ISN) GO TO 50
      IF(ICARD1 .EQ. IC) GO TO 60
      WRITE(6,10) ISN, IC, ICARD
      STOP
C  FOUND *SN, READ DESCRIPTIONS FOR STREAMS
   50 CALL RSTRMN
C  RETURN FROM RSTRMN OCCURS ONLY WHEN A DATA CONTROL CARD
C  HAS BEEN ENCOUNTERED.  THE NEXT CARD SHOULD BE *C
      CALL RCARD
      IF(ICARD1 .EQ. IC) GO TO 60
      WRITE(6,30) IC, ICARD
      STOP
C  FOUND *C, READ CONFIGURATION
   60 CALL RCONFG
C  RETURN FROM RCONFG IS ONLY WHEN A DATA CONTROL CARD HAS
C  BEEN ENCOUNTERED. NEXT CARD SHOULD BE *OF OR *PR
      CALL RCARD
      IF(ICARD1 .EQ. IOF) GO TO 70
```

```
      IF(ICARD1 .EQ. IPR) GO TO 90
      WRITE(6,10) IOF, IPR, ICARD1
      STOP
C  FOUND *OF, READ OFF-LINE PARAMETER LIST
   70 CALL OFLINE
      OFF= .TRUE.
C  RETURN FROM OFLINE IS ONLY WHEN A DATA CONTROL CARD HAS
C  BEEN ENCOUNTERED. NEXT CARD SHOULD BE *PR, *PL, OR *RUN
      CALL RCARD
      IF(ICARD1 .EQ. IPR) GO TO 90
      IF(ICARD1 .EQ. IPL) GO TO 100
      IF(ICARD1 .EQ. IRUN) GO TO 120
      WRITE(6,80) IPR, IPL, IRUN, ICARD
   80 FORMAT('0*****EXPECTING ''',A4,''', ''',A4,''', OR '''
     & A4,''', FOUND'/' ''',20A4,'''')
      STOP
C  FOUND *PR, READ PRINT SPECIFICATIONS
   90 CALL RPRINT
C  RETURN FROM RPRINT IS ONLY WHEN A DATA CONTROL CARD HAS
C  BEEN ENCOUNTERED.  IT SHOULD BE *PL, *OL, OR *RUN
      CALL RCARD
      IF(ICARD1 .EQ. IPL) GO TO 100
      IF(ICARD1 .EQ. IOL) GO TO 110
      IF(ICARD1 .EQ. IRUN) GO TO 120
      WRITE(6,80) IPL, IOL, IRUN, ICARD
      STOP
C  FOUND *PL, READ PLOT SPECIFICATIONS
  100 CALL PLOT1
C  RETURN FROM PLOT1 IS ONLY WHEN A DATA CONTROL CARD HAS
C  BEEN ENCOUNTERED.  NEXT CARD SHOULD BE *OL OR *RUN
      CALL RCARD
      IF(ICARD1 .EQ. IOL) GO TO 110
      IF(ICARD1 .EQ. IRUN) GO TO 120
      WRITE(6,10) IOL, IRUN, ICARD
      STOP
C  FOUND *OL, LOCATE THE OLD VALUES
  110 CALL OLDVAL
      GO TO 150
C  FOUND *RUN, READ RUN PARAMETERS
  120 READ(5,130) FTIME, DT
  130 FORMAT(2F10.0)
      IF(OFF) WRITE(8,140) FTIME, DT
  140 FORMAT(A4)
  150 WRITE(6,160) FTIME, DT
  160 FORMAT('1*RUN      RUN TIME PARAMETERS'/
     & 6X,'TOTAL TIME FOR RUN',G12.4,' HRS'/6X,
     & 'INTEGRATION STEP SIZE',G12.4,' HRS')
      CALL RCARD
      RETURN
      END
```

```
      SUBROUTINE RMCDPB
C
C  READ MODEL PARAMETERS
C
      REAL MWHOCL, MWOCL, L, NF, NTPIDT, KLA, KHENRY, KRATE,
     &     KDCOMP
      REAL*8 VHC, ALPHC, RDHC, KEQHC, CAOCL2, DTHC
C  LABELED COMMON STATEMENTS FOR REVERSE-OSMOSIS UNITS
      COMMON /PARMRO/ L, RO, RI, DF, TOLMX, TOLMN, KWRITE,
     &                NSTEPS
      COMMON /ROFIT / AKA, AKC, ERE, APIRO, BPIRO, GAMARO,
     &                BRO, CRO, NF, ROKE
      COMMON /ROPARM/ TEMP, VISC, DELP, RHOB, MCNT2, MCNT3,
     &                JWRITE
C  LABELED COMMON STATEMENTS FOR OZONE UNITS
      COMMON /UVFIT/  KHENRY, ECOZ, ETOC, KRATE, KDCOMP,
     &                EOZD, UVEFCT, ALPHA, EN, QPRIME
      COMMON /UVPARM/ CAREA, PAREA, UVH, UVRHO, UVPRES,
     &                UVTEMP, NWRITE
      COMMON /GASLAW/ RGAS
C  LABELED COMMON STATEMENTS FOR ULTRAFILTRATION MODULE
      COMMON /UFPARM/ PLENUF, DTUBUF, NTUF, JPUFSS, JWUFSS
      COMMON /PARMUF/ TEMPUF, VISCUF, DENBUF, ZREOUF, DROPUF
      COMMON /UFSAV1/ NSTPUF
      COMMON /UFFIT / G1UF, G2UF, GINFUF, C1, C2, CINF
C  LABELED COMMON STATEMENTS FOR TUBULAR R-O MODULE
      COMMON /TRPARM/ PLENTR, DTUBTR, NTTR, JPTRSS, JWTRSS
      COMMON /PARMTR/ TEMPTR, VISCTR, DENBTR, ZEROTR, DROPTR
      COMMON /TRFIT/  G1TR, G2TR, GINFTR, APITR, BTR, CTR,
     &                DCXTR, ADAXTR, BDAXTR, CDAXTR
C  LABELED COMMON STATEMENTS FOR GEL-MODEL
      COMMON /GMPARM/ PLENGM, DTUBGM, NTGM, JPGMSS, JWGMSS
      COMMON /PARMGM/ TEMPGM, VISCGM, DENBGM, ZEROGM, DROPGM
      COMMON /GMFIT/  GAMMA, APIGM, BPIGM, BGM, CGM, RATIO,
     &                DCXGM, ADAXGM, BDAXGM, CDAXGM, CAGEL
C  LABELED COMMON STATEMENTS FOR HYPOCHLORINATION MODULE
      COMMON /HCPARM/ VHC, ALPHC, RDHC, KEQHC, CAOCL2,
     &                JWRTHC, MCNTHC
      COMMON /HCSAV2/ MWHOCL, MWOCL, HCRHO
      DIMENSION JCARD(20), IUNIT(8)
      NAMELIST /NAMERO/ TOLMX, TOLMN, MCNT2, MCNT3, KWRITE,
     &                  AKA, AKC, ERE, APIRO, BPIRO, GAMARO,
     &                  BRO, CRO, NF, ROKE, JWRITE, NSTEPS,
     &                  VISC, RHOB
      NAMELIST /NAMEUV/ KHENRY, ECOZ, ETOC, KRATE, KDCOMP,
     &                  EOZD, UVEFCT, ALPHA, EN, QPRIME,
     &                  NWRITE, RGAS, UVRHO
      NAMELIST /NAMEUF/ JPUFSS, JWUFSS, G1UF, G2UF, GINFUF,
     &                  C1, C2, CINF, VISCUF, DENBUF
      NAMELIST /NAMETR/ JPTRSS, JWTRSS, G1TR, G2TR, GINFTR,
     &                  APITR, BTR, CTR, DCXTR, ADAXTR,
     &                  BDAXTR, CDAXTR, VISCTR, DENBTR
      NAMELIST /NAMEGM/ JPGMSS, JWGMSS, GAMMA, APIGM, BPIGM,
```

```
     &                       BGM, CGM, RATIO, DCXGM, ADAXGM,
     &                     BDAXGM, CDAXGM, CAGEL, VISCGM, DENBGM
      NAMELIST /NAMEHC/ ALPHC, RDHC, KEQHC, JWRTHC,
     &                       MCNTHC, MWHOCL, MWOCL, HCRHO
      DATA IUNIT/'NONE','*','UF','TR','GM','RO','UV','HC'/
   10 READ(5,20) ICARD,JCARD
   20 FORMAT(A4,T1,20A4)
      DO 30 I=1,8
      IF(ICARD .EQ. IUNIT(I))
     & GO TO (10, 110, 50, 60, 70, 80, 90, 100),I
C              NONE   *    UF  TR  GM  RO  UV   HC
   30 CONTINUE
      WRITE(6,40) JCARD
   40 FORMAT('THE FOLLOWING CARD IS INVALID AND WILL BE',
     & ' IGNORED'/1X,20A4)
      GO TO 10
   50 READ(5,NAMEUF)
      GO TO 10
   60 READ(5,NAMETR)
      GO TO 10
   70 READ(5,NAMEGM)
      GO TO 10
   80 READ(5,NAMERO)
      GO TO 10
   90 READ(5,NAMEUV)
      GO TO 10
  100 READ(5,NAMEHC)
      GO TO 10
  110 WRITE(6,120)
  120 FORMAT('1*MP       MODEL PARAMETERS'/)
C
      WRITE(6,130)
  130 FORMAT('0MODEL PARAMETERS FOR ULTRAFILTRATION MODULE')
      ICARD=0
      WRITE(6,140) JPUFSS, G1UF, G2UF, GINFUF, JWUFSS, C1,
     &              C2, CINF, VISCUF, DENBUF
  140 FORMAT('0 JPUFSS=',I3,'     G1UF=',G12.5,'    G2UF=',
     & G12.5,'  GINFUF=',G12.5/'  JWUFSS=',I3,'      C1=',
     & G12.5,'       C2=',G12.5,'    CINF=',G12.5/12X,
     &      '  VISCUF=',G12.5,'  DENBUF=',G12.5)
C
      WRITE(6,150)
  150 FORMAT('0MODEL PARAMETERS FOR TUBULAR RO MODULE')
      WRITE(6,160) JPTRSS, G1TR, G2TR, GINFTR,JWTRSS,ADAXTR,
     &              BDAXTR, CDAXTR, APITR, BTR, CTR, DCXTR,
     &              VISCTR, DENBTR
  160 FORMAT('0 JPTRSS=',I3,'     G1TR=',G12.5,'    G2TR=',
     &G12.5,'  GINFTR=',G12.5/'  JWTRSS=',I3,'  ADAXTR=',
     & G12.5,'  BDAXTR=',G12.5,'  CDAXTR=',G12.5/15X,
     & 'APITR=',G12.5,'     BTR=',G12.5,'      CTR=',G12.5/
     & 15X,'DCXTR=',G12.5,'  VISCTR=',G12.5,'  DENBTR=',
     & G12.5)
C
      WRITE(6,170)
```

```
  170 FORMAT('OMODEL PARAMETERS FOR GEL-MODEL')
      WRITE(6,180) JPGMSS, GAMMA, APIGM, BPIGM, JWGMSS, BGM,
     &             CGM, RATIO, DCXGM, ADAXGM, BDAXGM,
     &             CDAXGM, CAGEL, VISCGM, DENBGM
  180 FORMAT('0 JPGMSS=',I3,'   GAMMA=',G12.5,'   APIGM=',
     & G12.5,'   BPIGM=',G12.5/'  JWGMSS=',I3,'     BGM=',
     & G12.5,'     CGM=',G12.5,'   RATIO=',G12.5/15X,
     & 'DCXGM=',G12.5,'  ADAXGM=',G12.5,'  BDAXGM=',G12.5/
     &  14X,'CDAXGM=',G12.5,'   CAGEL=',G12.5,'  VISCGM=',
     & G12.5/14X,'DENBGM=',G12.5)
C
      WRITE(6,190)
  190 FORMAT('OMODEL PARAMETERS FOR REVERSE OSMOSIS')
      WRITE(6,200) JWRITE, TOLMX, TOLMN, AKA, MCNT2, AKC,
     &             ERE, APIRO, MCNT3, BPIRO, GAMARO, BRO,
     &             NSTEPS, CRO, NF, ROKE, KWRITE, VISC,
     &             RHOB
  200 FORMAT('0 JWRITE=',I3,'   TOLMX=',G12.5,'   TOLMN=',
     & G12.5,'     AKA=',G12.5/'   MCNT2=',I3,'     AKC=',
     &G12.5,'     ERE=',G12.5,'   APIRO=',G12.5/'   MCNT3=',
     & I3,'   BPIRO=',G12.5,'  GAMARO=',G12.5,'     BRO=',
     & G12.5/'  NSTEPS=',I3,'     CRO=',G12.5,'      NF=',
     & G12.5,'    ROKE=',G12.5/'  KWRITE=',I3,'    VISC=',
     & G12.5,'    RHOB=',G12.5)
C
      WRITE(6,210)
  210 FORMAT('OMODEL PARAMETERS FOR THE UV/OZONATION UNIT')
      WRITE(6,220) NWRITE, KHENRY, ECOZ, ETOC, KRATE,
     &             KDCOMP, EOZD, UVEPCT, ALPHA, EN, QPRIME,
     &             RGAS, UVRHO
  220 FORMAT('0 NWRITE=',I3,'  KHENRY=',G12.5,'    ECOZ=',
     & G12.5,'    ETOC=',G12.5/15X,'KRATE=',G12.5,
     & '  KDCOMP=',G12.5,'    EOZD=',G12.5/14X,'UVEPCT=',
     & G12.5,'   ALPHA=',G12.5,'      EN=',G12.5/14X,
     & 'QPRIME=',G12.5,'    RGAS=',G12.5,'   UVRHO=',G12.5)
C
      WRITE(6,230)
  230 FORMAT('OMODEL PARAMETERS FOR HYPOCHLORINATION UNIT')
      WRITE(6,240) JWRTHC, ALPHC, RDHC, HCRHO, MCNTHC,
     &             KEQHC, CAOCL2, MWHOCL, MWOCL
  240 FORMAT('0 JWRTHC=',I3,'   ALPHC=',G12.5,'    RDHC=',
     & G12.5,'   HCRHO=',G12.5/'  MCNTHC=',I3,'   KEQHC=',
     & G12.5,'  CAOCL2=',G12.5,'  MWHOCL=',G12.5/15X,
     & 'MWOCL=',G12.5)
      RETURN
      END
```

```
      SUBROUTINE RSTRME
C
C  READ STREAM ELEMENT DEFINITIONS
C
      COMMON STREAM(4,100), ICCNFG(8,100), PAR(500), NPAR,
     &       NCALL, IUNIT, NFATER, NS, NEQ, DESC(5)
      COMMCN /CREAD/ IFIRST, IAST, ICARD(20)
      COMMON /NAMES/ IUNITS(12), NMSTRM(5,100),
     &               NMEQPT(5,100), NMELE(5,5), ISUNIT(5),
     &               NMPAR(6,75), IDNMPH(150)
      DIMENSION L(5)
      WRITE(6,10)
   10 FORMAT('1*SE      STREAM ELEMENT DEFINITIONS'//6X,
     & 'ELEMENT   UNITS        DESCRIPTION')
   20 READ(5,30) IFIRST, NS1, K, L, ICARD
   30 FORMAT(A1,I4,1X,A4,5X,5A4,T1,20A4)
C  IF FIRST CHARATER IS "*" THEN A CONTROL CARD WAS FOUND
      IF(IFIRST .EQ. IAST) RETURN
      IF(NS1 .LE. 0 .OR. NS1 .GT. 5) GO TO 60
      ISUNIT(NS1)= K
      DO 40 J= 1,5
   40 NMELE(NS1,J) = L(J)
      WRITE(6,50) NS1, ISUNIT(NS1), (NMELE(NS1,J), J= 1,5)
      GO TO 20
   50 FORMAT(1X,I9,6X,A4,5X,10A4)
   60 WRITE(6,70) NS1, ICARD
   70 FORMAT('0*****ELEMENT',I3,' ENCOUNTERED.  WE ONLY HAVE
     & ' ELEMENTS ONE THROUGH FIVE (1-5). CHECK DATA CARD.'/
     & ' ''',20A4,'''')
      STOP
      END
```

```
      SUBROUTINE RSTRMN
C
C  READ THE NAMES OF THE STREAMS
C
      COMMON /CREAD/ IFIRST, IAST, ICARD(20)
      COMMON /NAMES/ IUNITS(12), NMSTRM(5,100),
     &               NMECPT(5,100), NMELE(5,5), ISUNIT(5),
     &               NMPAR(6,75), IDNMPR(150)
      DIMENSION L(5)
      WRITE(6,10)
   10 FORMAT('1*SN      STREAM NAMES'//6X,'STREAM      ',
     & 'DESCRIPTION')
   20 READ(5,30) IFIRST, N, L, ICARD
   30 FORMAT(A1,I4,5X,5A4,T1,20A4)
C  IF FIRST CHARACTER IS "*" THEN A CONTROL CARD WAS READ
      IF(IFIRST .EQ. IAST) RETURN
      DO 40 J=1,5
   40 NMSTRM(J,N)= L(J)
      WRITE(6,50) N,(NMSTRM(J,N),J=1,5)
   50 FORMAT(1X,I9,5X,5A4)
      GO TO 20
      END
```

```
      SUBROUTINE RCONFG
C
C  READ PLANT CONFIGURATION
C
      INTEGER NPAREQ(18), NPARIC(18), EQNAME(4,18)
      COMMON STREAM(4,100), ICONFG(8,100), PAR(500), NPAR,
     &       NCALL, IUNIT, NPATER, NS, NEQ, DESC(5)
      COMMON /CREAD/ IFIRST, IAST, ICARD(20)
      COMMON /NAMES/ IUNITS(12), NMSTRM(5,100),
     &               NMEQPT(5,100), NMELE(5,5), ISUNIT(5),
     &               NMPAR(6,75), IDNMPR(150)
C  NPAREQ(I) IS THE NUMBER OF PARAMETERS FOR EQUIPMENT TYPE
      DATA NPAREQ/4, 6, 1, 1, 7, 0, 6, 6, 12, 8, 0, 7, 4, 5,
     &            5, 6, 6, 6/
C  NPARIC(I) IS THE NUMBER OF INITIAL CONDITIONS FOR
C   EQUIPMENT TYPE I
      DATA NPARIC/4, 4, 6*0, 3, 5,8*0/
      DATA EQNAME/'MIXE', 'D TA', 'NK  ', '    ',
     &            'OVER', 'FLOW', ' TAN', 'K   ',
     &            'PUMP', '    ', '    ', '    ',
     &            'STRE', 'AM S', 'PLIT', 'TER ',
     &            'STRE', 'AM S', 'OURC', 'E   ',
     &            'STRE', 'AM M', 'IXER', '    ',
     &            'ULTR', 'AFIL', 'TRAT', 'ION ',
     &            'REVE', 'RSE ', 'OSMO', 'SIS ',
     &            'UV-O', 'ZONE', ' UNI', 'T   ',
     &            'HYPO', 'CHLO', 'RINA', 'TION',
     &            'STRE', 'AM S', 'INK ', '    ',
     &            'PID ', 'CONT', 'ROLL', 'ER  ',
     &            'SENS', 'OR  ', '    ', '    ',
     &            'MANI', 'PULA', 'TOR ', '    ',
     &            'RATI', 'O CO', 'NTRO', 'LLER',
     &            'BINA', 'RY C', 'ONTR', 'OLER',
     &            'TUBU', 'LAR ', 'R-O ', '    ',
     &            'GEL ', 'MODE', 'L UF', '    '/
      WRITE(6,10)
   10 FORMAT('1*C       PLANT CONFIGURATION'/)
       NCALL= -1
        NPAR= 1
       IUNIT=1
   20 READ(5,30) IFIRST, (ICONFG(I,IUNIT), I= 1,7),
     &            (NMEQPT(I,IUNIT), I= 1,5), ICARD, DESC
   30 FORMAT(A1,I4,3X,A2,5I5,5X,5A4,T1,20A4,T41,5A4)
C  IF FIRST CHARACTER IS "*" THEN A CONTROL CARD WAS FOUND
      IF(IFIRST .EQ. IAST) GO TO 60
         NEQ= IUNIT
      ICONFG(8,IUNIT)= NPAR
C CHANGE EQUIPMENT TYPE ALPHA CODE TO NUMERIC CODE
      CALL EQCODE
C
C READ AND WRITE THE PARAMETERS ASSOCIATED WITH EACH UNIT OF
C     EQUIPMENT.
C
```

```
C READ INPUT CATA
        ITYPE= ICONFG(2,IUNIT)
        NPARS= NPAREQ(ITYPE)
        NPARF= NPAR + NPARS - 1
      IF(NPARS .EQ. 0) NPARF= NPAR
      READ(5,40) (PAR(I), I= NPAR, NPARF)
   40 FORMAT(8E10.0)
      WRITE(6,50) ICONFG(1,IUNIT), (EQNAME(J,ITYPE), J= 1, 4
     &            DESC
   50 FORMAT('0UNIT NC.',I5,10X,4A4,4X,10A4)
C  CALL PRNTEQ TO PRINT OUT STREAM INPUTS AND OUTPUTS FOR
C          UNIT IUNIT
      CALL PRNTEQ(NPARIC(ITYPE))
      WRITE(6,30)
        NPAR= NPAR + NPARS
       IUNIT= IUNIT + 1
      GC TO 20
   60    NEQ= IUNIT - 1
      CALL STRM2
      IF(NFATER .EQ. 0) RETURN
      WRITE(6,70) NFATER
   70 FORMAT('0*****',I5,' FATAL ERRORS.  RUN TERMINATED.')
      STOP
      END
```

```
      SUBROUTINE STRM1
C
C  THIS SUBROUTINE IS USED TO MAKE SURE THAT NO STREAM HAS
C  BEEN GIVEN A MULTIPLE DEFINITION
C
      COMMON STREAM(4,100), ICONFG(8,100), PAR(500), NPAR,
     &       NCALL, IUNIT, NFATER, NS, NEQ, DESC(5)
      COMMON /CHECK/ JSCK(2,100)
      DO 110 I= 3,7
         K= ICONFG(I,IUNIT)
      IF(K) 60, 120, 10
C  AN INPUT STREAM
   10 IF(JSCK(1,K)) 40, 20, 30
   20 JSCK(1,K)= ICCNFG(1,IUNIT)
      GO TO 110
   30 JSCK(1,K) = -JSCK(1,K)
   40    L= IABS(JSCK(1,K))
      WRITE(6,50) K, L
   50 FCRMAT(6X,'*****STREAM',I4,' HAS BEEN PREVIOUSLY',
     & ' DEFINED AS AN INPUT TO UNIT',I4)
      NFATER= NFATER + 1
      GO TO 110
C  AN OUTPUT STREAM
   60    K= -K
      IF(JSCK(2,K)) 90, 70, 80
   70 JSCK(2,K)= ICONFG(1,IUNIT)
      GO TO 110
   80 JSC (2,K) = -JSCK(2,K)
   90    L= IABS(JSCK(2,K))
       E(6,100) K, L
  100 .  MAT(6X,'*****STREAM',I4,' HAS BEEN PREVIOUSLY',
     & ' DEFINED AS AN OUTPUT FROM UNIT',I4)
      NFATER= NFATER + 1
  110 CONTINUE
  120 RETURN
      END
```

```
      SUBROUTINE STRM2
C
C PRINT STREAM SUMMARY
C
      COMMON STREAM(4,100), ICONFG(8,100), PAR(500), NPAR,
     &       NCALL, IUNIT, NFATER, NS, NEQ, DESC(5)
      COMMCN /CHECK/ JSCK(2,100)
      WRITE(6,10)
   10 FORMAT('1STREAM SUMMARY'/6X,'STREAM',5X,'SOURCE',
     & 5X,'DESTINATICN')
      DC 210 I= 1,100
           K= JSCK(1,I)
           L= JSCK(2,I)
      IF(L) 20, 90, 140
   20      L= -L
      IF(K) 30, 50, 70
   30      K=  -K
      WRITE(6,40) I, L, K
   40 FORMAT(1X,I9,I11,I14,5X,'SOURCE AND DESTINATION',
     & ' MULTIPLE DEFINITION')
      NFATER= NFATER + 1
      GO TO 210
   50 WRITE(6,60) I, L, K
   60 FORMAT(1X,I9,I11,I14,5X,'SOURCE MULTIPLE DEFINITIONS'/
     & ' NO DESTINATION DEFINITION')
      NFATER= NFATER + 1
      GO TO 210
   70 WRITE(6,80) I, L, K
   80 FORMAT(1X,I9,I11,I14,5X,'SOURCE MULTIPLE DEFINITIONS')
      NFATER= NFATER + 1
      GO TO 210
   90 IF(K) 100, 210, 120
  100      K= -K
      WRITE(6,110) I, L, K
  110 FORMAT(1X,I9,I11,I14,5X,'NO SOURCE DEFINITION/MULTIPLE
     1DEFINITIONH')
      NFATER= NFATER + 1
      GC TO 210
  120 WRITE(6,130) I, L, K
  130 FORMAT(1X,I9,I11,I14,5X,'NO SOURCE DEFINITION')
      NFATER= NFATER + 1
      GO TO 210
  140 IF(K) 150, 170, 190
  150      K= -K
      WRITE(6,160) I, L, K
  160 FORMAT(1X,I9,I11,I14,5X,'MULTIPLE DESTINATION DEFINITI
      NFATER= NFATER + 1
      GC TC 210
  170 WRITE(6,180) I, L, K
  180 FORMAT(1X,I9,I11,I14,5X,'NO DESTINATION DEFINITION')
      NFATER= NFATER + 1
      GO TO 210
  190 WRITE(6,200) I, L, K
```

```
200 FORMAT(1X,I9,I11,I14)
210 CONTINUE
    RETURN
    END
```

```
      SUBROUTINE EQCCDE
C
C  CHANGE EQUIPMENT TYPE ALPHA CODE TO NUMBERIC CODE
C
      COMMON STREAM(4,100), ICONFG(8,100), PAR(500), NPAR,
     &       NCALL, IUNIT, NFATER, NS, NEQ, DESC(5)
C  EQUIPMENT CODE ARRAY
      DIMENSION ICODE(18)
      DATA ICODE /'MT', 'OT', 'P ', 'SP', 'SO', 'SM', 'UF',
     &            'RO', 'UV', 'HC', 'SK', 'CN','SN','MN',
     &            'RC', 'BC', 'TR', 'GM'/
C  GET EQUIPMENT CODE FOR UNIT "IUNIT"
           M= ICONFG(2,IUNIT)
C  LOCK IN EQUIPMENT CODE TABLE
      DO 10 I=1,18
      IF(M .EQ. ICODE(I)) GO TO 40
   10 CONTINUE
C  WE DID NOT FIND CODE IN TABLE
      WRITE(6,20) M, (ICONFG(I,IUNIT), I= 1,7)
   20 FORMAT(/' *****EQUIPMENT CODE ',A2,' IN FOLLOWING',
     & ' ENTRY IS ILLEGAL'/11X,I5,3X,A2,5I5/)
      NFATER= NFATER + 1
      ICONFG(2,IUNIT)= 0
      READ(5,30) A
   30 FORMAT(A4)
      RETURN
C  SET EQUIPMENT TYPE EQUAL TO NUMBERIC CODE
   40 ICONFG(2,IUNIT)= I
      RETURN
      END
```

```
      SUBROUTINE PRNTEQ(NINCON)
C
C  PRINT THE SPECIFICATIONS
C
      COMMON STREAM(4,100), ICONFG(8,100), PAR(500), NPAR,
     &        NCALL ,IUNIT, NFATER, NS, NEQ, DESC(5)
      COMMON /NAMES/ IUNITS(12), NMSTRM(5,100),
     &                NMEQPT(5,100), NMELE(5,5), ISUNIT(5),
     &                NMPAR(6,75), IDNMPR(150)
      INTEGER ISTR(5), OSTR(5)
C  STREAM CONTAINS THE INFORMATION FOR EACH STREAM
C  ICONFG CONTAINS THE INFORMATION FOR EACH UNIT
C  NINCON IS THE NUMBER OF INITIAL CONDITIONS
C  NINSTR IS THE NUMBER OF INPUT STREAMS (MAX= 5)
C  NOTSTR IS THE NUMBER OF OUTPUT STREAMS (MAX= 5)
      NINSTR= 0
      NOTSTR= 0
C  POSITIONS 3 THRU 7 OF ICONFG CONTAIN THE STREAM NUMBERS
C   TO/FROM UNIT IUNIT
      DO 30 I=3,7
           J= ICONFG(I,IUNIT)
      IF(J) 10, 30, 20
   10 NOTSTR= NOTSTR + 1
      OSTR(NOTSTR) = -J
      GO TO 30
   20 NINSTR= NINSTR + 1
      ISTR(NINSTR) = J
   30 CONTINUE
      WRITE(6,40)
   40 FORMAT(6X,'INPUT  STREAMS')
      IF(NINSTR .NE. 0) GO TO 60
      WRITE(6,50)
   50 FORMAT(11X,'NONE')
      GO TO 90
   60 DO 70 I= 1,NINSTR
           J= ISTR(I)
   70 WRITE(6,80) J, (NMSTRM(K,J), K= 1,5)
   80 FORMAT(1X,I15,5X,5A4)
   90 WRITE(6,100)
  100 FORMAT(6X,'OUTPUT STREAMS')
      IF(NOTSTR .NE. 0) GO TO 110
      WRITE(6,50)
      GO TO 130
  110 DO 120 I=1,NOTSTR
           J= OSTR(I)
  120 WRITE(6,80) J, (NMSTRM(K,J), K=1,5)
C  CALL STRM1 TO CHECK FOR CONSISTANCY
  130 CALL STRM1
C  POSITION 2 OF ICONFG CONTAINS THE TYPE CODE FOR UNIT IUNI
         KEQ= ICONFG(2,IUNIT)
           K= 1
  140 IF(IDNMPR(K) .EQ. KEQ) GO TO 150
           K= K + 2 + IDNMPR(K+1)
```

```
      GO TO 140
  150 KPAR= IDNMPR(K+1)
             K= K + 2
             L= NPAR
      WRITE(6,160)
  160 FORMAT( 6X,'INITIAL CONDITIONS')
      IF(NINCON .NE. 0) GO TO 180
      WRITE(6,170)
  170 FORMAT( 11X,'NONE')
      GO TO 210
  180 DO 200 I=1,NINCON
             J= IDNMPR(K)
      M= NMPAR(6,J)
      WRITE(6,190) (NMPAR(IA,J), IA=1,5), PAR(L), IUNITS(M)
  190 FORMAT(11X,5A4,G14.5,1X,A4)
             L= L + 1
  200        K= K + 1
  210 WRITE(6,220)
  220 FORMAT( 6X,'DESIGN PARAMETERS')
      NDESPR= KPAR - NINCON
      IF(NDESPR .NE. 0) GO TO 230
      WRITE(6,170)
      RETURN
  230 DO 240 I=1,NDESPR
             J= IDNMPR(K)
             M= NMPAR(6,J)
      WRITE(6,190) (NMPAR(IA,J), IA=1,5), PAR(L), IUNITS(M)
             L= L + 1
  240        K= K + 1
      RETURN
      END
```

```
      SUBROUTINE RPRINT
C
C  READ PRINT SPECIFICATIONS
C
      COMMON /CPRINT/ TPRINT, NPELE, KPRINT(2,10)
      WRITE(6,10)
   10 FORMAT('1*PR      PRINT SPECIFICATIONS'/)
      READ(5,20) TPRINT
   20 FORMAT(G10.5)
      WRITE(6,30) TPRINT
   30 FORMAT('0      PRINT INTERVAL IS ',G13.5,' HRS'/)
      CALL SPEC(KPRINT,NPELE,10)
      RETURN
      END
```

```
      SUBROUTINE OFLINE
C
C  SETUP THE LABEL ON THE OFF-LINE STARAGE DEVICE (UNIT 8)
C
      COMMON /CTIME/ TIME, FTIME, DT
      COMMON /COFLN/ NPL, LIST(2,50), LABLE, TOFLN,
     &               MESSAG(20), IEOF, IHEAD
      WRITE(6,10)
   10 FORMAT('1*OL      OFF-LINE PARAMETER LIST')
      READ(5,20) MESSAG
   20 FORMAT(20A4)
      WRITE(6,30) MESSAG
   30 FORMAT(' THE HEADER MESSAGE FOR THE DATA SET IS'/
     & 1X,20A4)
      READ(5,40) LABLE
   40 FORMAT(I2)
      IF(LABLE .LT. 0) GO TO 60
      WRITE(6,50)
   50 FORMAT(' THE NEW VALUES WILL BE ADDED TO THE END',
     & ' OF THE DATA SET.')
      GO TO 80
   60 WRITE(6,70)
   70 FORMAT(' THE DATA SET WILL BE CLEARED, AND THE NEW',
     & ' VALUES SAVED FROM THE BEGINNING.')
   80 READ(5,90) TOFLN
   90 FORMAT(F10.3)
      WRITE(6,100) TOFLN
  100 FORMAT(' THE SAVE INTERVAL IS',G12.4)
      CALL SPEC(LIST,NPL,50)
C
C  WRITE LABEL ON OFF-LINE STORAGE DEVICE ON UNIT 8
C
C IF LABLE .LT. 0, THEN CLEAR DATA SET
C IF LABLE .GE. 0, THEN ADD AT THE END OF THE DATA SET
      REWIND 8
      IF(LABLE .LT. 0) GO TO 120
  110 READ(8,150,END=130) ICODE
      IF(ICODE .NE. IEOF) GO TO 110
      BACKSPACE 8
C  WRITE HEADER
  120 WRITE(8,150) IHEAD, MESSAG, TOFLN, NPL,
     &            (LIST(1,I), LIST(2,I), I= 1, NPL)
      RETURN
  130 WRITE(6,140)
  140 FORMAT(' ***** END-OF-FILE OCCURRED WHILE SETTING',
     & ' UP THE OFF-LINE STORAGE HEADER *****')
      STOP
  150 FORMAT(A4)
      END
```

```
      SUBROUTINE PLOT1
C
C  READ IN THE PARAMETERS/ELEMENTS TO PLOT
C
      COMMON /CPLOT/ NPLOT, TPLOT, KPLOT, PLTDTA(100,10),
     &               JPSTRM(2,10)
      READ(5,10) TPLOT
   10 FORMAT(F10.0)
      WRITE(6,20)
   20 FORMAT('1*PL       PLOT VARIABLES')
      WRITE(6,30) TPLOT
   30 FORMAT(/6X, 'PLOT DURATION', F7.2, ' HRS'/)
      CALL SPEC(JPSTRM,NPLOT,10)
      RETURN
      END
```

```
      SUBROUTINE OLDVAL
C
C  LOCATE THE DESIRED SET OF OLD VALUES
C
      COMMON /COFLN/ NPL, LIST(2,50), IABLE, TOFLN,
     &               MESSAG(20), IEOF, IHEAD
      COMMON /CTIME/ TIME, FTIME, DT
      DIMENSION MSG(20)
      WRITE(6,1)
    1 FORMAT('1*OL           OLD VALUES SPECIFICATIONS')
C  READ THE UNIQUE MESSAGE
      READ(5,10) MESSAG
   10 FORMAT(20A4)
      WRITE(6,20) MESSAG
   20 FORMAT(1X,20A4)
      REWIND 8
C  FIND HEADER
   30 READ(8,70,END=50) ICODE
      IF(ICODE .EQ. IEOF) GO TO 50
      IF (ICODE .NE. IHEAD) GO TO 30
      READ(8,70,END=50) MSG
      DO 40 I=1,20
      IF(MSG(I) .NE. MESSAG(I)) GO TO 30
   40 CONTINUE
      READ(8,70,END=50) TOFLN, NPL, (LIST(1,I), LIST(2,I),
     &                  I= 1, NPL), FTIME, DT
         NPL= -NPL
      RETURN
   50 WRITE(6,60) MESSAG
   60 FORMAT(' THE RUN FOR'/1X,20A4/' WAS NOT FOUND.')
      STOP
   70 FORMAT(A4)
      END
```

```
      SUBROUTINE SAVEIT
C
C  SAVE VALUES CN OFF-LINE STORAGF DEVICE, UNIT 8
C
      COMMON /COFLN/ NPL, LIST(2,50) , LABLE, TOFLN,
     &              MESSAG(20), IEOF, IHEAD
      COMMON STREAM(4,100), ICONFG(8,100), PAR(500), NPAR,
     &        NCALL, IUNIT, NFATER, NS, NEQ, DESC(5)
      COMMON /CTIME/ TIME, FTIME, DT
      DIMENSICN P(50)
      IF(NPL .LE. 0) RETURN
      DO 20 I= 1, NPL
           K= LIST(1,I)
           L= LIST(2,I)
      IF(K .GT. 0) GO TO 10
        P(I)= PAR(L)
      GO TO 20
   10   P(I)= STREAM(L,K)
   20 CONTINUE
      WRITE(8,30) TIME, (P(I),I=1,NPL)
   30 FORMAT(A4)
      RETURN
      END
```

```
      SUBROUTINE GETIT
C
C  RETREIVE THE VALUES THAT WERE SAVED ON THE OFF-LINE
C    STORAGE DEVICE, UNIT 8, BY "SAVEIT" IN A PREVIOUS RUN
C
      COMMON /COFLN/ NPL, LIST(2,50) , IABLE, TOFLN,
     &                 MESSAG(20), IEOF, IHEAD
      COMMON STREAM(4,100), ICONFG(8,100), PAR(500), NPAR,
     &         NCALL, IUNIT, NPATER, NS, NEQ, DESC(5)
      COMMON /CTIME/ TIME, FTIME, DT
      DIMENSION P(50)
      KPL= -NPL
      READ(8,30) TIME, (P(J),J=1,KPL)
      DO 20 I= 1, KPL
           K= LIST(1,I)
           L= LIST(2,I)
      IF(K .GT. 0) GO TO 10
      PAR(L)= P(I)
      GO TO 20
   10 STREAM(L,K)= P(I)
   20 CONTINUE
   30 FORMAT(A4)
      RETURN
      END
```

```
      SUBROUTINE PRINT
C
C  THIS SUBROUTINE IS USED TO PRINT OUT THE SPECIFIED VALUES
C
      COMMON STREAM(4,100), ICONFG(8,100), PAR(500), NPAR,
     &       NCALL, IUNIT, NFATER, NS, NEQ, DESC(5)
      COMMON /CPRINT/ TPRINT, NPELE, KPRINT(2,10)
      COMMON /CTIME/ TIME, FTIME, DT
      DIMENSION P(10), NME1(10), NME2(10), I1(10), I2(10),
     &          NAME1(2), NAME2(2)
      DATA NAME1, NAME2/'STRM', 'UNIT', 'ELE.', 'PAR.'/
      DATA LINE, NLINES/0, 51/
C  PRINT HEADINGS WHEN LINE = 0
      IF(LINE .GT. 0) GO TO 50
      DO 20 I= 1, NPELE
           K= KPRINT(1,I)
           L= KPRINT(2,I)
           J= 1
      IF(K .GT. 0) GO TO 10
           J= 2
           K= -K
           L= L - ICONFG(8,K) + 1
           K= ICONFG(1,K)
   10 NME1(I)= NAME1(J)
      NME2(I)= NAME2(J)
        I1(I)= K
   20   I2(I)= L
      WRITE(6,30) (NME1(I), I1(I), I= 1, NPELE)
   30 FORMAT('1',10X,10(4X,A4,I4))
      WRITE(6,40) (NME2(I), I2(I), I= 1, NPELE)
   40 FORMAT(6X,'TIME ',10(4X,A4,I4))
        LINE= NLINES
C  RETRIEVE ELEMENTS
   50 DO 70 I= 1, NPELE
           K= KPRINT(1,I)
           L= KPRINT(2,I)
      IF(K .GT. 0) GO TO 60
        P(I)= PAR(L)
      GO TO 70
   60   P(I)= STREAM(L,K)
   70 CONTINUE
      WRITE(6,80) TIME, (P(I), I= 1, NPELE)
   80 FORMAT(1X,G10.3,10G12.3)
        LINE= LINE - 1
      RETURN
      END
```

```
      SUBROUTINE PLOT2
C
C  SAVE THE VALUES OF THE PARAMETERS/ELEMENTS FOR PLOTTING
C
       COMMON STREAM(4,100), ICONFG(8,100), PAR(500), NPAR,
     &        NCALL, IUNIT, NFATER, NS, NEQ, DESC(5)
      COMMON /CPLOT/ NPLOT, TPLOT, KPLOT, PLTDTA(100,10),
     &               JPSTRM(2,10)
      COMMON /CTIME/ TIME, FTIME, DT
      IF(KPLOT .EQ. 100) RETURN
   10 CONTINUE
       KPLOT= KPLOT + 1
      DO 30 I= 1, NPLOT
           K= JPSTRM(1,I)
           L= JPSTRM(2,I)
      IF(K .GT. 0) GO TO 20
      PLTDTA(KPLOT,I)= PAR(L)
      GO TO 30
   20 PLTDTA(KPLOT,I)= STREAM(L,K)
   30 CONTINUE
      IF(KPLOT*0.01*TPLOT .LE. TIME) GO TO 10
      RETURN
      END
```

```
      SUBROUTINE SPEC (IARRAY,N,NZ)
C
C  READ VARIABLES TO BE PRINTED, PLOTTED, OR SAVED OFF-LINE
C
      COMMON  STREAM(4,100), ICONFG(8,100), PAR(500), NPAR,
     1        NCALL, IUNIT, NFATER, NS, NEQ, DESC(5)
      COMMON /CREAD/ IFIRST, IAST, ICARD(20)
      COMMON /NAMES/ IUNITS(12), NMSTRM(5,100),
     &               NMEQPT(5,100), NMELE(5,5), ISUNIT(5),
     &               NMPAR(6,75), IDNMPR(150)
      DIMENSION IARRAY(2,NZ)
            N=0
   10 READ(5,20) IFIRST, K, L, ICARD
   20 FORMAT(A1,I4,I5,T1,20A4)
C  IF THE FIRST CHARACTER IS '*' THEN IT IS A CONTROL CARD
      IF(IFIRST .EQ. IAST) RETURN
      IF(N .LT. NZ) GO TO 40
      WRITE(6,30) ICARD, NZ
   30 FORMAT(' *****CARD ''',20A4,''' IGNORED.',I4,
     & ' MAXIMUM')
      GO TO 10
   40 IF(K .GT. 0) GO TO 110
C ENTRY IS UNIT/PARAMETER
            K= -K
C LOOK FOR UNIT NUMBER IN CONFIGURATION ARRAY
      DO 50 I= 1,NEQ
      IF(ICONFG(1,I) .EQ. K) GO TO 70
   50 CONTINUE
      WRITE(6,60) ICARD, K
   60 FORMAT(' *****CARD ''',20A4,''' IGNORED.  NO UNIT',
     & ' NUMBER',I5)
      GO TO 10
C WE HAVE FOUND UNIT K
   70       N= N + 1
      IARRAY(1,N)= -I
      IARRAY(2,N)= ICONFG(8,I) + L - 1
      ITYPE= ICONFG(2,I)
            M= 1
   80 IF(IDNMPR(M) .EQ. ITYPE) GO TO 90
            M= M + 2 + IDNMPR(M+1)
      GO TO 80
   90       M= M + 1 + L
            M= IDNMPR(M)
      WRITE(6,100) K, (NMEQPT(J,I), J= 1,5), L,
     &              (NMPAR(J,M), J= 1,5)
  100 FORMAT(' +++++UNIT', I9, 5X, 5A4 / 6X, 'PARAMETER',
     & I4, 6X, 5A4)
      GO TO 10
C ENTRY IS STREAM/ELEMENT
  110       N= N + 1
      IARRAY(1,N)= K
      IARRAY(2,N)= L
      WRITE(6,120) K, (NMSTRM(J,K), J= 1, 5), L,
```

```
     &               (NMELE(L,J), J= 1, 5)
 120 FORMAT(' -----STREAM', 17, 5X, 5A4 / 6X,
     & 'ELEMENT', I6, 5X, 5A4)
      GC TC 10
      END
```

```
      SUBROUTINE RCARD
C
C  READ A DATA CONTROL CARD
C
      COMMON /CREAD/ IFIRST, IAST, ICARD(20)
      READ(5,10) IFIRST, ICARD
   10 FORMAT(A1,T1,20A4)
C  FIRST CHARACTER MUST BE '*' FOR A DATA CONTROL CARD
      IF(IFIRST .EQ. IAST) RETURN
      WRITE(6,20) ICARD
   20 FORMAT('0*****EXPECTING DATA CONTROL CARD, FOUND '/
     & ' ''',20A4,'''')
      STOP
      END
```

```
      SUBROUTINE SUBCAL
C     CALL SUBROUTINE CORRESPONDING TO EQUIPMENT TYPE
      COMMON STREAM(4,100), ICONFG(8,100), PAR(500), NPAR,
     &       NCALL, IUNIT, NFATER, NS, NEQ, DESC(5)
C     GET EQUIPMENT TYPE
      ITYPE= ICONFG(2,IUNIT)
      IF(ITYPE .EQ. 0) RETURN
      GO TO(10,20,30,40,50,60,70,80,90,100,110,120,130,140,
C          MT OT  P SP SO SM UF RO UV  HC  SK  CN  SN  MN
     &     150,160,170,180),ITYPE
C           RC  BC  TR  GM
      RETURN
   10 CALL MT
      RETURN
   20 CALL OT
      RETURN
   30 CALL P
      RETURN
   40 CALL SP
      RETURN
   50 CALL SO
      RETURN
   60 CALL SM
      RETURN
   70 CALL UF
      RETURN
   80 CALL RO
      RETURN
   90 CALL UV
      RETURN
  100 CALL HC
      RETURN
  110 CALL SK
      RETURN
  120 CALL PID
      RETURN
  130 CALL SENSOR
      RETURN
  140 CALL MANIP
      RETURN
  150 CALL RATIO
      RETURN
  160 CALL BINARY
      RETURN
  170 CALL TR
      RETURN
  180 CALL GM
      RETURN
      END
```

```
      SUBROUTINE PLOT3
C
C  THIS SUBROUTINE MAKES THE LINEPRINTER PLOTS
C
      COMMON STREAM(4,100), ICONFG(8,100), PAR(500), NPAR,
     &       NCALL, IUNIT, NFAIER,NS,NEQ,DESC(5)
      COMMON /CPLOT/ NPLOT, TPLOT, KPLOT, PLTDTA(100,10),
     &               JPSTRM(2,10)
      COMMON /CREAD/ IFIRST, IAST, ICARD(20)
      COMMON /NAMES/ IUNITS(12), NMSTRM(5,100),
     &               NMEQPT(5,100), NMELE(5,5), ISUNIT(5),
     &               NMPAR(6,75), IDNMPR(150)
      DIMENSION ICHR(10), IARR(100), XAXIS(5), PLTCRD(2,10)
      EQUIVALENCE (ICARD1,ICARD(1))
      DATA ICD1/'*PC '/, IBLK/' '/, ISTAR/'*'/
      IF(NPLOT .EQ. 0) RETURN
          K1= 1
      CALL RCARD
      IF(ICARD1 .EQ. ICD1) GO TO 20
      WRITE(6,10) ICARD
   10 FORMAT('0EXPECTING DATA CONTROL CARD ''*PC '', FOUND'/
     &       ' ''',20A4,'''')
      STOP
   20 WRITE(6,30)
   30 FORMAT('1PLOT PARAMETERS')
      DO 100 K2= K1, NPLOT
      READ(5,40) ICHR(K2), (PLTCRD(J,K2), J= 1, 2)
   40 FORMAT(A1,4X,2F10.0)
      IF(ICHR(K2) .EQ. IBLK) GO TO 110
          K= JPSTRM(1,K2)
          L= JPSTRM(2,K2)
      IF(K .GT. 0) GO TO 80
          K= -K
      IUNIT= ICONFG(2,K)
        KPAR= L - ICONFG(8,K) + 1
          M= 1
   50 IF(IDNMPR(M) .EQ. IUNIT) GO TO 60
          M= M + 2 + IDNMPR(M+1)
      GO TO 50
   60     M= M + 1 + KPAR
         MI= IDNMPR(M)
        IXYZ= K
        JXYZ= ICONFG(1,K)
      WRITE(6,70) ICHR(K2), JXYZ, (NMEQPT(J,IXYZ), J=1,5),
     &            PLTCRD(1,K2), KPAR,
     &            (NMPAR(J,MI),J=1,5), PLTCRD(2,K2)
   70 FORMAT(/1X,A1,'----UNIT',I10,5X,5A4,5X,'YO    =',F12.2/
     1 6X,'PARAMETER',I5,5X,5A4,5X,'YMAX =',F12.2)
      GO TO 100
   80 WRITE(6,90) ICHR(K2), K, (NMSTRM(J,K),J=1,5),
     &            PLTCRD(1,K2), L,
     &            (NMELE(L,J),J=1,5),PLTCRD(2,K2)
   90 FORMAT(/1X,A1,'----STREAM',I8,5X,5A4,5X,'YO    =',
```

```
     & F12.2/6X,'ELEMENT',I7,5X,5A4,5X,'YMAX =',F12.2)
 100 CONTINUE
          K2= NPLOT
     GO TO 120
 110      K2= K2 - 1
 120 WRITE(6,130)
 130 FORMAT('0')
       LINE= 40
 140 DO 150 I=1,100
 150 IARR(I)= IBLK
           K= K2
 160      YO= PLTCRD(1,K)
         YMX= PLTCRD(2,K)
          DY= (YMX-YO)/40.
     DO 170 I= 1, KPLOT
           J= 0.5 + (PLTDTA(I,K)-YO)/DY
     IF(J .NE. LINE) GO TO 170
      ICHAR= ICHR(K)
     IF(IARR(I) .NE. IBLK) ICHAR= ISTAR
     IARR(I)= ICHAR
 170 CONTINUE
           K= K - 1
     IF(K .GE. K1) GO TO 160
     IF((LINE/10)*10 .EQ. LINE) GO TO 190
     WRITE(6,180) IARR
 180 FORMAT(11X,'*',100A1)
     GO TO 210
 190      YO= PLTCRD(1,K1)
         YMX= PLTCRD(2,K1)
          DY= (YMX-YO)/40.
          YC= YO + LINE*DY
     WRITE(6,200) YC, IARR
 200 FORMAT(1X,F10.2,'+',100A1)
 210   LINE= LINE - 1
          YO= PLTCRD(1,K1)
     IF(LINE .NE. 0) GO TO 140
     WRITE(6,220) YO
 220 FORMAT(1X,F10.2,'+',10('*********+'))
          DX= TPLOT/5.
     DO 230 I=1,5
 230 XAXIS(I)= DX*I
     WRITE(6,240) XAXIS
 240 FORMAT(10X,'0.00',5F20.2//50X,'TIME, HR '/)
          K1= K2 + 1
     IF(K1 .LE. NPLOT) GO TO 20
     CALL RCARD
     RETURN
     END
```

```
      SUBROUTINE MT
C
C  THIS SUBROUTINE SIMULATES A MIXING TANK
C
C                         _______________
C           INPUT     |                 |  OUTPUT
C          STREAMS    |     MIXING      |  STREAMS
C        ---------->|      TANK       |---------->
C        ---------->|_________________|---------->
C
C  PARAMETER          QUANTITY
C      1              INITIAL VOLUME
C      2              INITIAL TSS CONC.
C      3              INITIAL TDS CONC.
C      4              INITIAL TOC CONC.
C
      COMMON STREAM(4,100), ICONFG(8,100), PAR(500), NPAR,
     &        NCALL, IUNIT, NFATER, NS, NEQ, DESC(5)
      COMMON /CTIME/  TIME, FTIME, DT
      COMMON /MATBAL/ BALNCE(4), AMTIN(4), AMTOUT(4)
      COMMON /LOOK/   ISW
C  ASCERTAIN IF READ PARAMETERS, INITIALIZE, OR COMPUTE
      IF(NCALL) 10, 20, 70
C  MATERIAL BALANCE
   10 BALNCE(1)= PAR(NPAR)  + BALNCE(1)
      BALNCE(2)= PAR(NPAR)*PAR(NPAR+1)  + BALNCE(2)
      BALNCE(3) = PAR(NPAR)*PAR(NPAR+2)  + BALNCE(3)
      BALNCE(4) = PAR(NPAR)*PAR(NPAR+3)  + BALNCE(4)
      RETURN
C  INITIALIZATION CALCUALTIONS
   20 DO 50 I= 3, 7
             J= ICONFG(I,IUNIT)
      IF(J) 30, 60, 50
   30        J= -J
      STREAM(2,J)= PAR(NPAR+1)
      STREAM(3,J)= PAR(NPAR+2)
      STREAM(4,J) = PAR(NPAR+3)
   50 CONTINUE
   60 RETURN
C     SIMULATION
   70        V= PAR(NPAR)
           VC2= V*PAR(NPAR+1)
           VC3= V*PAR(NPAR+2)
           VC4= V*PAR(NPAR+3)
      DO 100 I=3,7
             J= ICONFG(I,IUNIT)
      IF(J) 80, 100, 90
C  OUTPUT STREAM
   80        J= -J
             F= STREAM(1,J)
           TSS= PAR(NPAR+1)
           TDS= PAR(NPAR+2)
           TOC= PAR(NPAR+3)
```

```
      STREAM(2,J) = TSS
      STREAM(3,J)= TDS
      STREAM(4,J)= TOC
           V= V - DT*F
         VC2= VC2 - DT*F*TSS
         VC3= VC3 - DT*F*TDS
         VC4= VC4 - DT*F*TOC
      GO TO 100
C  INPUT STREAM
   90      F= STREAM(1,J)
           V= V + DT*F
         VC2= VC2 + DT*F*STREAM(2,J)
         VC3= VC3 + DT*F*STREAM(3,J)
         VC4= VC4 + DT*F*STREAM(4,J)
  100 CONTINUE
      IF(V .GT. 0.0) GO TO 130
      WRITE(6,110) ICONFG(1,IUNIT)
  110 FORMAT('0*****WARNING. UNIT NUMBER',I5,' HAS RUN DRY')
      DO 120 J= 1, 4
  120 PAR(NPAR+J-1) = 0.
      GO TO 140
  130 CONTINUE
        PAR(NPAR)= V
      PAR(NPAR+1)= VC2/V
      PAR(NPAR+2)= VC3/V
      PAR(NPAR+3)= VC4/V
  140 CONTINUE
           J= NPAR + 3
      IF(ISW.EQ.1) WRITE(6,150) IUNIT,(PAR(I),I=NPAR,J)
  150 FORMAT(' UNIT',I5,' MT  VOL=',G10.3,5X,'SS=',
     &  G10.3,5X,'DS=',G10.3,
     & 'TOC=',G10.3)
      GO TO 20
      END
```

```
      SUBROUTINE OT
C
C  THIS SUBROUTINE SIMULATES AN OVERFLOW TANK
C
C                      _____________
C            INPUT    |             | OVERFLOW
C           STREAMS   |  OVERFLOW   |----------> 1
C         --------->|     TANK     |  OUTPUT
C         --------->|_____________|---------->
C
C  PARAMETER        QUANTITY
C       1           INITIAL VOLUME
C       2           INITIAL TSS CONC.
C       3           INITIAL TDS CONC.
C       4           INITIAL TOC CONC.
C       5           OVERFLOW RATE
C       6           MAXIMUM VOLUME
C
C  THE OVERFLOW STREAM MUST BE SPECIFIED FIRST
      COMMCN STREAM(4,100), ICONFG(8,100), PAR(500), NPAR,
     &       NCALL, IUNIT, NFATER, NS, NEQ, DESC(5)
      COMMON /CTIME/  TIME, FTIME, DT
      COMMCN /MATBAL/ BALNCE(4), AMTIN(4), AMTOUT(4)
      COMMCN /LCCK/   ISW
C ASCERTAIN IF READ PARAMETERS, INITIALIZE, OR SIMULATE
      IF(NCALL) 10,60,110
   10 IF(ICONFG(3,IUNIT).LT.0) GOTO30
      WRITE(6,20) IUNIT,ICONFG(3,IUNIT)
   20 FORMAT(6X,'*****ERROR, UNIT',I5,'. FIRST STREAM IN',
     & ' CONFIGURATION IS',I5,'. MUST BE THE OUTPUT STREAM',
     & ' FOR OVERFLOW')
      NFATER= NFATER + 1
   30 IF(PAR(NPAR+5) .GT. 0.) GO TO 50
      WRITE(6,40) IUNIT, PAR(NPAR+5)
   40 FORMAT(6X,'*****ERROR, UNIT',I5,'.  MAXIMUM VOLUME =',
     & F10.2,' IS INVALID.  MUST BE POSITIVE.')
      NFATER= NFATER + 1
C  MATERIAL BALANCE
   50 BALNCE(1)= PAR(NPAR)  + BALNCE(1)
      BALNCE(2)= PAR(NPAR)*PAR(NPAR+1)  + BALNCE(2)
      BALNCE(3)= PAR(NPAR)*PAR(NPAR+2)  + BALNCE(3)
      BALNCE(4)= PAR(NPAR)*PAR(NPAR+3)  + BALNCE(4)
      RETURN
C  INITIALIZATION CALCULATIONS
   60       J=-ICONFG(3,IUNIT)
      STREAM(1,J)= PAR(NPAR+4)
   70 DO 90 I= 3, 7
            J= ICONFG(I,IUNIT)
      IF(J) 80,100,90
   80       J= -J
      STREAM(2,J)= PAR(NPAR+1)
      STREAM(3,J)= PAR(NPAR+2)
      STREAM(4,J)= PAR(NPAR+3)
```

```
 90 CONTINUE
100 RETURN
C  SIMULATION
110       F= 0.
    DO 140 I= 4, 7
          J= ICONFG(I,IUNIT)
    IF(J) 120,140,130
120       J= -J
          F= F - STREAM(1,J)
    GO TO 140
130       F= F + STREAM(1,J)
140 CONTINUE
          V= PAR(NPAR)
          K= -ICONFG(3,IUNIT)
       FLOW= PAR(NPAR+4)
         VX= V + (F-FLOW)*DT
       VMAX= PAR(NPAR+5)
    IF(VX .GT. VMAX) FLOW= (V + F*DT - VMAX)/DT
    IF(VX .LT. 0.) FLOW= (V + F*DT)/DT
    STREAM(1,K)= FLOW
    PAR(NPAR)= V + (F - FLOW)*DT
        VC2= V*PAR(NPAR+1)
        VC3= V*PAR(NPAR+2)
        VC4= V*PAR(NPAR+3)
    DO 170 I= 3, 7
          J= ICONFG(I,IUNIT)
    IF(J) 150, 170, 160
C  OUTPUT STREAM
150       J= -J
    STREAM(2,J)= PAR(NPAR+1)
    STREAM(3,J)= PAR(NPAR+2)
    STREAM(4,J)= PAR(NPAR+3)
          F= STREAM(1,J)
    IF(F .LT. 1.E-20)F=0.
        VC2= VC2 - DT*F*STREAM(2,J)
        VC3= VC3 - DT*F*STREAM(3,J)
        VC4= VC4 - DT*F*STREAM(4,J)
    GO TO 170
C  INPUT STREAM
160       F= STREAM(1,J)
    IF(F .LT. 1.E-20) F= 0.
        VC2= VC2 + DT*F*STREAM(2,J)
        VC3= VC3 + DT*F*STREAM(3,J)
        VC4= VC4 + DT*F*STREAM(4,J)
170 CONTINUE
         VF= PAR(NPAR)
    IF(VF .LT. 1.E-20) GO TO 180
    PAR(NPAR+1)= VC2/VF
    PAR(NPAR+2)= VC3/VF
    PAR(NPAR+3)= VC4/VF
180 CONTINUE
          J= NPAR + 3
    IF(ISW .EQ. 1) WRITE(6,190) IUNIT,(PAR(I),I=NPAR,J)
190 FORMAT(' UNIT',I5,' OT  VOL=',G10.3,5X,'SS=',G10.3,5X,
```

```
& 'DS=',G10.3,'TOC=',G10.3)
 GO TO 70
 END
```

```
      SUBROUTINE P
C
C  SIMULATION OF VOLUMETRIC PUMP
C
C                              _____________
C              INPUT     |             | OUTPUT
C              STREAM    | VOLUMETRIC  | STREAM
C           1 -------->|    PUMP     |--------> 2
C                        |_____________|
C
C  PARAMETER        QUANTITY
C      1            FLOW RATE
C
C  THE INPUT STREAM MUST BE SPECIFIED FIRST
C  THE OUTPUT STREAM MUST BE SPECIFIED SECOND
      COMMON /LOOK/ ISW
      COMMON STREAM(4,100), ICONFG(8,100), PAR(500), NPAR,
     &       NCALL, IUNIT, NPATER, NS, NEQ, DESC(5)
C  ASCERTAIN IF READ DATA, INITIALIZE, OR SIMULATE
      IF(NCALL) 10, 20, 20
C RETURN IF MATERIAL BALANCE CALCULATIONS
   10 RETURN
C     INITIALIZE AND SIMULATE ARE IDENTICAL
   20           K= ICONFG(3,IUNIT)
                L= -ICONFG(4,IUNIT)
      STREAM(1,K) = PAR(NPAR)
      STREAM(1,L)= PAR(NPAR)
      STREAM(2,L)= STREAM(2,K)
      STREAM(3,L)= STREAM(3,K)
      STREAM(4,L)= STREAM(4,K)
      IF(ISW .EQ. 1) WRITE(6,30) IUNIT,(STREAM(I,L),I=1,4)
   30 FORMAT(' UNIT',I5,' P   FLOW=',G10.3,5X,'SS=',
     & G10.3,5X,'DS=',G10.3,5X,'TOC=',G10.3)
      RETURN
      END
```

```
      SUBROUTINE SP
C
C     SIMULATION OF STREAM SPLITTER
C
C                   _____________
C          INPUT   |             | OUTPUT
C         STREAM   |   STREAM    | STREAMS
C       1 ------->|   SPLITTER  |--------> 2 SPECIFIED
C                  |_____________|--------> 3 DIFFERENCE (1-2)
C
C  PARAMETER       QUANTITY
C      1           FLOW RATE OF STREAM 2
C
C  THE FEED STREAM MUST BE SPECIFIED FIRST
C  THE SPECIFIED STREAM MUST BE SECOND
C  THE DIFFERENCE STREAM MUST BE THIRD
      COMMON /LOCK/ ISW
      COMMON STREAM(4,100), ICONFG(8,100), PAR(500), NPAR,
     &       NCALL, IUNIT, NFATER, NS, NEQ, DESC(5)
C     ASCERTAIN IF READ DATA, INITIALIZE, OR SIMULATE
      IF(NCALL) 10, 20, 20
C  RETURN IF MATERIAL BALANCE CALCULATIONS
   10 RETURN
C     INITIALIZE AND SIMULATE ARE IDENTICAL
C  STREAM J IS THE INPUT
C  STREAM K IS THE SPECIFIED OUTPUT
C  STREAM L IS THE DIFFERENCE BETWEEN J AND K
   20            J= ICONFG(3,IUNIT)
                 K= -ICONFG(4,IUNIT)
                 L= -ICONFG(5,IUNIT)
                F1= STREAM(1,J)
                F2= PAR(NPAR)
      IF(F1 .LT. F2) F2= F1
      STREAM(1,K)= F2
      STREAM(1,L)= F1 - F2
      DO 30 I=2,4
      STREAM(I,L) = STREAM(I,J)
   30 STREAM(I,K)= STREAM(I,J)
      IF(ISW.EQ.1) WRITE(6,40) IUNIT,F2,(STREAM(I,L),I=1,4)
   40 FORMAT(' UNIT',I5,' SP FLOW1=',G10.3,5X,'FLOW2=',G10.3
     &  5X,'SS=',G10.3,5X,'DS=',G10.3,5X,'TOC=',G10.3)
      RETURN
      END
```

```
      SUBROUTINE SO
C
C  SIMULATION OF STREAM SOURCE
C
C
C                         ___________
C                        |           | OUTPUT
C                        |  STREAM   | STREAM
C                        |  SOURCE   |---------> 1
C                        |___________|
C
C  PARAMETER        QUANTITY
C      1            TIME OF FIRST PULSE
C      2            PULSE WIDTH
C      3            CYCLE TIME
C      4            FLOW RATE
C      5            TSS CONC.
C      6            TDS CONC.
C      7            TOC CCN.
      COMMON /LOOK/   ISW
      COMMON  STREAM(4,100),ICONFG(8,100),PAR(500),NPAR,
     &        NCALL, IUNIT, NFATER, NS, NEQ, DESC(5)
      COMMON /CTIME/  TIME, FTIME, DT
      COMMON /MATBAL/ BALNCE(4), AMTIN(4), AMTOUT(4)
C  ASCERTAIN IF READ DATA, INITIALIZE, OR SIMULATE
      IF(NCALL) 10, 20, 20
C  ERROR CHECK
   10          J= -ICONFG(3,IUNIT)
      IF(J .GT. 0) RETURN
      WRITE(6,21) IUNIT, J
   21 FORMAT(' ****IN UNIT',I4,', SO, OUTPUT STREAM IS',
     & ' SPECIFIED AS AN INPUT STREAM (',I3,')')
      NFATER= NFATER + 1
      RETURN
C  INITIALIZE AND SIMULATE ARE IDENTICAL
   20          J= -ICONFG(3,IUNIT)
      STREAM(2,J) = PAR(NPAR+4)
      STREAM(3,J) = PAR(NPAR+5)
      STREAM(4,J)= PAR(NPAR+6)
              TE= TIME - PAR(NPAR)
              TE= TE + DT
             TCY= PAR(NPAR+2)
             NCY= TE/TCY + 0.0001
              TR= TE - TCY*NCY
      IF(TE .LT. 0.) GO TO 50
C     IF(TR .LT. PAR(NPAR+1)) GO TO 60
      IF(TR .LE. PAR(NPAR+1)) GO TO 40
      IF((TR-DT) .GT. PAR(NPAR+1)) GO TO 30
           FRACT= (PAR(NPAR+1) - (TR-DT))/DT
      GO TO 70
   30      FRACT= 0.
      GO TO 70
   40      FRACT= TR/DT
      GO TO 70
```

```
   50 STREAM(1,J)= 0.
      GO TO 90
C  60 STREAM(1,J)= PAR(NPAR+3)
   70 CONTINUE
      IF(FRACT .GT. 1.) FRACT= 1.
      IF(FRACT .LT. 0.0) FRACT= 0.
                 F= PAR(NPAR+3)*FRACT
      STREAM(1,J)= F
      IF(NCALL .EQ. 0) RETURN
C                F= STREAM(1,J)
         AMTIN(1)= AMTIN(1)  + F*DT
      DO 80 L=2,4
   80 AMTIN(L)= AMTIN(L)  + F*STREAM(L,J)*DT
   90 IF(ISW .EQ. 1) WRITE(6,100) IUNIT, (STREAM(I,J),I=1,4)
  100 FORMAT(' UNIT',I5,' SO  FLOW=',G10.3,5X,'SS=',
     &     G10.3,5X,'DS=',G10.3,5X,'TOC=',G10.3)
      RETURN
      END
```

```
      SUBBOUTINE SM
C
C   SIMULATION OF STREAM MIXER
C
C
C             INPUT    |            | OUTPUT
C           --------->|  STREAM    |
C           --------->|  MIXER     |--------->
C           --------->|____________|
C
C   NO PARAMETERS REQUIRED
C
C   OUTPUT STREAM MUST BE SPECIFIED LAST
C
      COMMCN /LCCK/ ISW
      CCMMCN STREAM(4,100), ICONFG(8,100), PAR(500), NPAR,
     &       NCALL, IUNIT, NFATER, NS, NEQ, DESC(5)
C   ASCERTAIN IF READ DATA, INITIALIZE, OR SIMULATE
      IF(NCALL) 10, 20, 20
C   RETURN IF MATERIAL BALANCE CALCULATICNS
   10 RETURN
C   INITIALIZE AND SIMULATE ARE IDENTICAL
   20            FJ= 0.
                  F= 0.
                FC4= 0.
                FC2= 0.
                FC3= 0.
      DC 30 I=3,7
                  J= ICONFG(I,IUNIT)
      IF(J .LT. 0) GO TO 40
                 FI= STRFAM(1,J)
                  F= F + FI
                FC2= FC2 + FI*STREAM(2,J)
                FC3= FC3 + FI*STREAM(3,J)
   30           FC4= FC4 + FI*STREAM(4,J)
   40             J= -J
      STREAM(1,J)= F
      IF(F .LT. 1.E-20) GO TO 50
      STREAM(2,J)= FC2/F
      STREAM(3,J)= FC3/F
      STREAM(4,J)= FC4/F
      GO TO 70
   50 CONTINUE
C   IF FLOW IS ZERO, SET CONCENTRATIONS ACCORDINGLY
      DO 60 I=2,4
   60 STREAM(I,J)= 0.
   70 CONTINUE
      IF(ISW .EQ. 1) WRITE(6,80) IUNIT,(STREAM(I,J),I=1,4)
   80 FORMAT(' UNIT',I5,' SM  FLOW=',G10.3,5X,'SS=',
     & G10.3,5X,'DS=',G10.3,5X,'TOC=',G10.3)
      RETURN
      END
```

```
      SUBROUTINE UF
C
C  ULTRAFILTRATION MODEL INTERFACE TO WPE SIMULATOR
C
C                          _________________   PERMEATE
C                         |                 |------------> 1
C       FEED              | ULTRAFILTRATION |
C   3 ---------->|                 |
C                         |     MODULE      | CONCENTRATE
C                         |_________________|------------> 2
C
C  PARAMETER          QUANTITY
C      1              NUMBER OF TUBES
C      2              OPERATING TEMPERATURE
C      3              PRESSURE DROP ACROSS THE MEMBRANE
C                     AT THE INLET
C      4              PRESSURE DROP DOWN THE TUBE
C      5              TUBE DIAMETER
C      6              TUBE LENGTH
C
C  THE PERMEATE STREAM MUST BE SPECIFIED FIRST
C  THE CONCENTRATE STREAM MUST BE SPECIFIED SECOND
C  THE FEED STREAM MUST BE SPECIFIED LAST
      REAL NTPIDT
      DIMENSION PERMN(100)
      COMMON /LOOK/ISW
      COMMCN STREAM(4,100), ICONFG(8,100), PAR(500), NPAR,
     &       NCALL, IUNIT, NFATER, NS, NEQ, DESC(5)
      COMMON /UFPARM/ PLEN, DTUBE, NT, JPRINT, JWRITE
      COMMON /PARMUF/ TEMP, VISC, DENB, DPZERO, PDROP
      IF(NCALL) 10, 80, 90
C  THERE ARE NO MATERIAL BALANCE CALCULATIONS.  HOWEVER,
C  THE STREAM SPECIFICATIONS ARE CHECKED FOR CONSISTENT
C  INPUT/OUTPUT
   10 CONTINUE
C  SOME ERROR CHECKING
      IF(ICONFG(3,IUNIT) .LT. 0) GO TO 30
      WRITE(6,20) IUNIT, ICONFG(3,IUNIT)
   20 FORMAT(6X,'*****ERROR, UNIT',I5,'.  FIRST STREAM IN ',
     & 'CONFIGURATION IS',I5,'.  MUST BE THE PERMEATE ',
     & '(OUTPUT).')
      NFATER= NFATER + 1
   30  IF(ICONFG(4,IUNIT) .LT. 0) GO TO 50
      WRITE(6,40) IUNIT,ICONFG(4,IUNIT)
   40 FORMAT(6X,'*****ERROR, UNIT',I5,'. SECOND STREAM IN ',
     & 'CONFIGURATION IS',I5,'.  MUST BE THE CONCENTRATE ',
     & '(OUTPUT).')
      NFATER= NFATER + 1
   50 IF(ICONFG(5,IUNIT) .GT. 0) GO TO 70
      WRITE(6,60) IUNIT,ICONFG(5,IUNIT)
   60 FORMAT(6X,'*****ERROR, UNIT',I5,'.  THIRD STREAM IN ',
     & 'CONFIGURATICN IS',I5,'.  MUST BE THE CONCENTRATE ',
     & '(OUTPUT).')
```

```
              NFATER= NFATER + 1
   70 CCNTINUE
         RETURN
   80 CONTINUE
C  INITIALIZATION SAME AS SIMULATE
         PERMN(IUNIT) = 0.
C        RETURN
   90 CCNTINUE
C  SET UP COMMON VARIABLES
                  NT= PAR(NPAR)
                TEMP= PAR(NPAR+1)
              DPZERO= PAR(NPAR+2)
               PDROP= PAR(NPAR+3)
               CTUBE= PAR(NPAR+4)
                PLEN= PAR(NPAR+5)
C  SIMULATE
               IPERM= -ICCNFG(3,IUNIT)
               ICCNC= -ICONFG(4,IUNIT)
               IFEED= ICONFG(5,IUNIT)
C  GET READY TO CALL UFSS
              KULTRA= -1
                  CS= STREAM(2,IFEED)
                  CD= STREAM(3,IFEED)
                  CC= STREAM(4,IFFED)
                FLOW= STREAM(1,IFEED)
                PERM= PERMN(IUNIT)
         IF(ISW .GE. 1)
        & WRITE(6,100) IPERM,ICONC,IFEED,CA,CC,FLOW
  100 FORMAT(' $$$ UF DEBUG',6G10.3)
         CALL UFSS(KULTRA,CS,CC,CC,FLOW,TOTALA,TOTALB,TOTALC,
        & PERM)
            PERMN(IUNIT) = PERM
                   TOTAL= TOTALA + TOTALB + TOTALC
         STREAM(3,IPERM) = TOTALA/TOTAL*DENB
         STREAM(4,IPERM) = TOTALC/TOTAL*DENB
         STREAM(1,IPERM) = TOTAL/DENB
C NO SUSPENDED SCLIDS PASS THROUGH UF MEMBRANE
         STREAM(2,IPERM) = 0.
C  CHECK FOR ERRORS
         IF(KULTRA .LT. 0) GO TO 120
         WRITE(6,110) KULTRA
  110 FORMAT(' *****ERROR IN UF WHILE CALLING UFSS. ',
        & ' KULTRA=',I5)
                 NFATER= NFATER + 1
  120 CONTINUE
C  GET FLOW RATE OF CONCENTRATE BY STEADY STATE MATERIAL
C   BALANCE
         STREAM(1,ICONC) = STREAM(1,IFEED) - STREAM(1,IPERM)
C  GET CONCENTRATICN OF CONCENTRATE BY COMPONENT BALANCE
         DO 130 I=2,4
         STREAM(I,ICONC) = (STREAM(I,IFEED)*STREAM(1,IFEED)-
        &    STREAM(I,IPERM)*STREAM(1,IPERM))/STREAM(1,ICONC)
  130 CONTINUE
         IF(ISW .EQ. 1) WRITE(6,140) IUNIT,(STREAM(I,IPERM),I=1
```

```
      & (STREAM(I,ICCNC),I=1,4)
  140 FORMAT(' UNIT',I5,' UF  PERM FLOW=',G10.3,5X,'SS=',
     &G10.3,5X,'DS=',G10.3,5X,'TOC=',G10.3/15X,'CONC FLOW=',
     &G10.3,5X,'SS=',G10.3,5X,'DS=',G10.3,5X,'TOC=',G10.3)
      RETURN
      END
```

```
      SUBROUTINE UFSS(KULTRA,SS,DS,TC,F,TOTALA,TOTALB,
     &                TOTALC,PERM)
C
C  THIS SUBROUTINE PERFORMS THE STEADY STATE CALCULATIONS FO
C     MULTIPLE TUBE ULTRAFILTRATION MODULES.
C  THIS ROUTINE ASSUMES COMPLETE REJECTION OF SUSPENDED SOLI
C    AND NO REJECTION OF DESOLVED SOLIDS.
C  SEE THE REPORT BY ABBOTT AND STERLING ON THE MODIFIED UF/
C    TUBULAR RO/ GEL MODEL FOR A DISCRIPTION OF VARIABLES
C
      REAL NTPIDT
      COMMON /UFPARM/ PLEN, DTUBE, NT, JPRINT, JWRITE
      COMMON /UFFIT/  GAM1, GAM2, GAMINF, C1, C2, CINF
      COMMON /PARMUF/ TEMP, VISC, DENB, DPZERO, PDROP
      COMMON /CTIME/  TIME, FTIME, DT
      DATA PIE/3.141593/
      NTPIDT= NT*DTUBE*PIE
      DPBAR= DPZERO - 0.5*PDROP
      GAMMA= GAMINF
      IF(GAM2*PERM .LT. 174.)
     & GAMMA= GAMINF + (GAM1-GAMINF)*EXP(-GAM2*PERM)
      TOTALB= PLEN*GAMMA*DPBAR*NTPIDT
      FB= (TOTALB/DENB)
      TOTALA= DS*FB
      TOTAL= TOTALA + TOTALB
      C= CINF
      IF(C2*PERM .LT. 174.) C= CINF + (C1 - CINF)*EXP(-C2*PE
      TOTALC= PLEN*NTPIDT*TC*TOTAL*C/(TOTAL + DENB*C)
      PERM= PERM + FB*DT
   10 IF(JPRINT .LE. 0) GO TO 50
      JPRINT= JPRINT - 1
      WRITE(6,20) SS,DS,TC,F,DPZERO,PDROP,PLEN,DT,DTUBE,NTPI
   20 FORMAT('      SS= ',G12.5,'      DS= ',G12.5,'      TC= '
     * '       F= ',G12.5/
     1 ' DPZERO= ',G12.5,'  PDROP= ',G12.5,'    PLEN= ',G12.5
     *,G12.5/
     2 '   DTUBE= ',G12.5,' NTPIDT= ',G12.5,'    DENB= ',G12.5
     3,G12.5)
      WRITE(6,30) GAM1,GAM2,GAMINF,C1,C2,CINF
   30 FORMAT('    GAM1= ',G12.5,'    GAM2= ',G12.5,' GAMINF= '
     * '       C1= ',G12.5,'       C2= ',G12.5,'    CINF= ',G12.5
      WRITE(6,40) DPBAR,GAMMA,C,PERM,TOTALA,TOTALB,TOTALC
   40 FORMAT(' DPBAR= ',G12.5,' GAMMA= ',G12.5,'        C= ',G
     1 '     PERM= ',G12.5/' TOTALA= ',G12.5,' TOTALB= ',G12.5
     2 ' TOTALC= ',G12.5)
   50 RETURN
      END
```

```
      SUBROUTINE UOZONE(ZINO,CZINO,TOCINO,G,F,ZOUT,CZOUT,
     &                  TOCOUT)
C
C  THIS SUBROUTINE PERFORMS THE STEADY STATE CALCULATIOS
C  FOR  THE ULTRAVIOLET OZONATION UNIT
C
      REAL KLA, KHENRY, KRATE, KDCOMP
      COMMON /DELTAT/ DT
      COMMON /UVL/    UVLITE
      COMMON /UVFIT/   KHENRY, ECOZ, ETOC, KRATE, KDCOMP,
     &                EOZD, UVEFCT, ALPHA, FN, QPRIME
      COMMON /UVPARM/ CAREA, PAREA, H, RHO, PRESS, TEMP, NWR
      DIMENSION ZOUT(10), CZOUT(10), TOCOUT(10), DCZBR(10),
     &          DTOCBR(10)
      COMMON /STAGES/ NSTAGE,PRECON
      DATA IFIRST/0/
      EQUIVALENCE (NNN,IEND)
         NNN= NSTAGE
      IF(PRECON .NE. 0.0) NNN= NSTAGE + 1
      IF(IFIRST .NE. 0) GO TO 20
C  FOR FIRST ITERATION, SET UP INLET GAS CONCENTRATION
C   TO PRE-CONTACTOR
      IFIRST= 1
       TZOUT= 0.
      DO 10 I= 1, NSTAGE
   10  TZOUT= TZOUT + ZOUT(I)
        ZBAR= TZOUT/NSTAGE
   20 CONTINUE
      UVLITE= 0.
C CALL FOR PRE-CONTACTOR
      CALL USTAGE(ZBAR, CZINO, TOCINO, NSTAGE*G, F,
     & ZOUT(NSTAGE+1), DCZBR(NSTAGE+1), DTOCBR(NSTAGE+1),
     & PAREA, CZOUT(NSTAGE+1), TOCOUT(NSTAGE+1))
       TZOUT= 0.
C SET UP UV RADIATION EFFECT ON REACTION RATE CONSTANTS
      UVLITE= UVEFCT
      DO 60 I= 1, NSTAGE
C SET UP INPUTS TO THE NEXT STAGE
         ZIN= ZINO
           N= I - 1
      IF(I .NE. 1) GO TO 30
           N= NSTAGE + 1
      IF(PRECON .EQ. 0.0) GO TO 40
   30 CONTINUE
        CZIN= CZOUT(N)
       TOCIN= TOCOUT(N)
      GO TO 50
   40 CONTINUE
        CZIN= CZINO
       TOCIN= TOCINO
   50 CONTINUE
      CALL USTAGE(ZIN, CZIN, TOCIN, G, F, ZOUT(I), DCZBR(I),
     & DTOCBR(I), CAREA, CZOUT(I), TOCOUT(I))
```

```
      TZOUT= TZOUT + ZOUT(I)
   60 CONTINUE
C DETERMINE NEXT GAS CONCENTRATION TO THE PRE-CONTACTOR
       ZBAR= TZOUT/NSTAGE
      DO 70 I= 1, IEND
C TAKE ONE INTEGRATION STEP
      CZOUT(I)= CZOUT(I) + DCZBR(I)*DT
   70 TOCOUT(I)= TOCOUT(I) + DTOCBR(I)*DT
      RETURN
      END
```

```
      SUBROUTINE GM
C
C  ULTRAFILTRATION GEL MODEL INTERFACE TO WPE SIMULATOR
C
C                       ________________   PERMEATE
C                      |                |------------> 1
C      FEED            |   GEL MODEL    |
C   3 --------->| ULTRAFILTRATION |
C                      |     MODULE     | CONCENTRATE
C                      |________________|------------> 2
C
C  PARAMETER         QUANTITY
C      1             NUMBER OF TUBES
C      2             OPERATING TEMPERATURE
C      3             PRESSURE DROP ACROSS THE MEMBRANE
C                    AT THE INLET
C      4             PRESSURE DROP DOWN THE TUBE
C      5             TUBE DIAMETER
C      6             TUBE LENGTH
C
C  THE PERMEATE STREAM MUST NE SPECIFIED FIRST
C  THE CONCENTRATE STREAM MUST BE SPECIFIED SECOND
C  THE FEED STREAM MUST BE SPECIFIED LAST
      REAL NTPIDT
      DIMENSION PERMN(100)
      COMMON /LCOK/ISW
      COMMON STREAM(4,100), ICONFG(8,100), PAR(500), NPAR,
     &       NCALL, IUNIT, NFATER, NS, NEQ, DESC(5)
      COMMON /GMPARM/ PLEN, DTUBE, NT, JPRINT, JWRITE
      COMMON /PARMGM/ TEMP, VISC, DENB, DPZERO, PDROP
      IF(NCALL) 10, 80, 90
   10 CONTINUE
C  THERE ARE NO MATERIAL BALANCE CALCULATIONS. HOWEVER, THE
C  STREAM SPECIFICATIONS ARE CHECKED FOR CONSISTENT
C  INPUT/OUTPUT
      IF(ICONFG(3,IUNIT) .LT. 0) GO TO 30
      WRITE(6,20) IUNIT, ICONFG(3,IUNIT)
   20 FORMAT(6X,'*****ERROR, UNIT',I5,'.  FIRST STREAM IN ',
     & 'CONFIGURATION IS',I5,'.  MUST BE THE PERMEATE ',
     & '(OUTPUT).')
      NFATER= NFATER + 1
   30 IF(ICONFG(4,IUNIT) .LT. 0) GO TO 50
      WRITE(6,40) IUNIT,ICONFG(4,IUNIT)
   40 FORMAT(6X,'*****ERROR, UNIT',I5,'. SECOND STREAM IN',
     & ' CONFIGURATION IS',I5,'.  MUST BE THE CONCENTRATE',
     & '  (OUTPUT).')
      NFATER= NFATER + 1
   50 IF(ICONFG(5,IUNIT) .GT. 0) GO TO 70
      WRITE(6,60) IUNIT,ICONFG(5,IUNIT)
   60 FORMAT(6X,'*****ERROR, UNIT',I5,'. THIRD STREAM IN',
     & ' CONFIGURATION IS',I5,'. MUST BE THE FEED ',
     & '  (INPUT).')
C  INCREMENT NUMBER OF FATAL ERRORS
```

```
         NFATER= NFATER + 1
      70 CONTINUE
         RETURN
      80 CONTINUE
C     INITIALIZATION SAME AS SIMULATE
         PERMN(IUNIT) = 0.
      90 CONTINUE
C     SET UP COMMON VARIABLES
             NT= PAR(NPAR)
           TEMP= PAR(NPAR+1)
         DPZERO= PAR(NPAR+2)
          PDROP= PAR(NPAR+3)
          DTUBE= PAR(NPAR+4)
           PLEN= PAR(NPAR+5)
C     SIMULATE
          IPERM= -ICONFG(3,IUNIT)
          ICONC= -ICONFG(4,IUNIT)
          IFEED= ICONFG(5,IUNIT)
C     GET READY TO CALL GMSS
         KULTRA= -1
             CS= STREAM(2,IFEED)
             CD= STREAM(3,IFEED)
             CC= STREAM(4,IFEED)
           FLOW= STREAM(1,IFEED)
           PERM= PERMN(IUNIT)
         IF(ISW .GE. 1)
        & WRITE(6,100) IPERM, ICONC, IFEED, CA, CC, FLOW
     100 FORMAT(' $$$ GM DEBUG',6G13.5)
         CALL GMSS(KULTRA,CS,CD,CC,FLOW,TOTALA,TOTALB,TOTALC,
        &          PERM)
           PERMN(IUNIT)= PERM
                  TOTAL= TOTALA + TOTALB + TOTALC
         STREAM(3,IPERM)= TOTALA/TOTAL*DENB
         STREAM(4,IPERM)= TOTALC/TOTAL*DENB
         STREAM(1,IPERM)= TOTAL/DENB
C NO SUSPENDED SOLIDS PASS THROUGH UF MEMBRANE
         STREAM(2,IPERM) = 0.
C     CHECK FOR ERRORS
         IF(KULTRA .LT. 0) GO TO 120
         WRITE(6,110) KULTRA
     110 FORMAT(' *****ERROR IN GEL WHILE CALLING GMSS.',
        & ' KULTRA=',I5)
         NFATER= NFATER + 1
     120 CONTINUE
C     GET FLOW RATE OF CONCENTRATE BY STEADY STATE MATERIAL
C     BALANCE
         STREAM(1,ICONC)= STREAM(1,IFEED) - STREAM(1,IPERM)
C     GET CONCENTRATION OF CONCENTRATE BY COMPONENT BALANCE
         DO 130 I=2,4
         STREAM(I,ICONC)= (STREAM(I,IFEED)*STREAM(1,IFEED)-
        &   STREAM(I,IPERM)*STREAM(1,IPERM))/STREAM(1,ICONC)
     130 CONTINUE
         IF(ISW .EQ. 1) WRITE(6,140) IUNIT,(STREAM(I,IPERM),I=1
        & (STREAM(I,ICONC),I=1,4)
```

```
140 FORMAT(' UNIT',I5,' GM  PERM FLOW=',G10.3,5X,'SS=',
   & G10.3,5X,'DS=',G10.3,5X,'TOC=',G10.3/15X,'CONC FLOW='
   & ,G10.3,5X,'SS=',G10.3,5X,'DS=',G10.3,5X,'TOC=',G10.3)
    RETURN
    END
```

```
      SUBROUTINE GMSS(KULTRA,SS,DS,TC,F,TOTALA,TOTALB,
     & TOTALC,PERM)
C
C  THIS SUBROUTINE PERFORMS THE STEADY STATE CALCULATIONS
C  FOR MULTIPLE TUBE ULTRAFILTRATION MODULES USING THE GEL
C    MODEL
C  THIS ROUTINE ASSUMES COMPLETE REJECTION OF SUSPENDED
C    SOLIDS
C  SEE THE REPORT BY ABBOTT AND STERLING ON THE MODIFIED UF/
C    TUBULAR RO/ GEL MODEL FOR A DISCRPTION OF VARIABLES
C
      REAL JA,JB,JC,NTPIDT
      COMMON /GMPARM/ PLEN, DTUBE, NT, JPRINT, JWRITE
      COMMON /PARMGM/ TEMP, VISC, DENB, DPZERO, PDROP
      COMMON /CTIME/  TIME, FTIME, DT
      DATA NSTEPS/10/
      DATA NDIM1/100/
          CA= DS
          CC= TC
          PI= 3.141593
C  DETERMINE AXIAL STEP SIZE FROM THE TUBE LENGTH AND
C  NUMBER OF INTEGRATION STEPS
          DZ= PLEN/NSTEPS
      NWRITE= 0
        AREA= 0.25*PI*DTUBE*DTUBE
      NTPIDT= NT*DTUBE*PI
      TOTALA= 0.
      TOTALB= 0.
      TOTALC= 0.
      DO 30 I=1,NSTEPS
           Z= (I-1)*DZ + 0.5*DZ
C  EVALUATE PRESSURE DROP AT MIDPOINT OF INTEGRATION STEP
        DELP= DPZERO - PDROP*Z/PLEN
           V= F/AREA
       KGETJ= 0
C  CALL GETJ TO GET THE FLUXES
      CALL GETJ(CA,CC,V,DELP,JA,JB,JC,KGETJ)
C  CALCULATE DERATIVES FOR THIS STEP
          DF= -NTPIDT*(JA + JB + JC)/DENB
        DFCA= -NTPIDT*JA
        DFCC= -NTPIDT*JC
C  PERFORM INTEGRATION
        FNEW= F + DF*DZ
          CA= (F*CA + DFCA*DZ)/FNEW
          CC= (F*CC + DFCC*DZ)/FNEW
C  UPDATE CUMULATIVE PERMEATE FLOWS OF A, B, AND C
      TOTALA= TOTALA + JA*NTPIDT*DZ
      TOTALB= TOTALB + JB*NTPIDT*DZ
      TOTALC= TOTALC + JC*NTPIDT*DZ
           F= FNEW
      IF(JPRINT .LE. 0) GO TO 30
C  DETERMINE IF ANY OUTPUT IS TO BE PRODUCED
      NWRITE= NWRITE + 1
```

```
      IF(NWRITE .LT. JPRINT) GO TO 30
      NWRITE= 0
      WRITE(6,20) I, Z, CA, CC, JA, JB, JC, F,
     &            TOTALA, TOTALB, TOTALC
   20 FORMAT(' STEP ',I4,'  Z= ',G13.5,'  CA= ',G13.5,
     &'  CC= ',G13.5/'  JA= ',G13.5,'  JB= ',G13.5,'  JC= ',
     & '  F= ',G13.5/'  TOTALA= ',G13.5,'  TOTALB= ',G13.5,
     & '  TOTALC= ',G13.5)
   30 CONTINUE
          DS= CA
          TC= CC
        PERM= PERM + (TOTALB/DENB)*DT
      IF(JPRINT .EQ. -999) WRITE(6,20) I, Z, CA, CC, JA, JB,
     &                        JC, F, TOTALA, TOTALB,TOTALC
      RETURN
      END
```

```
      SUBROUTINE GETJ(CA1,CC1,V,DELP,JA,JB,JC,KGETJ)
C
C  THIS IS THE GEL MODEL FOR THE ULTRAFILTRATION UNIT
C  SEE REPORT BY SMITH AND STARKS ON THE UF UNIT FOR A
C    DISCRIPTICN OF VARIABLES
C
      REAL NF, JA, JB, JC
      REAL*8 JB1, JB2, KA, KC, JDA, DAX, RE, SC, SH, CA2,
     &        CA2BIG, CA2SML, CA3, CA3BIG, CA3SML, PI,
     &        POSMOT, CEQ2, CEQ3, DELPI, PI2, PI3, CA3P,
     &        CA2P, XA1, XC1, CX, BX, CCGEL
      COMMON /GMPARM/ PLEN, DTUBE, NT, JPRINT, JWRITE
      COMMCN /PARMGM/ TEMP, VISC, DENB, DPZERO, PDROP
      COMMCN /GMFIT/  GAMMA, API, BPI, B, C, RATIO, DCX,
     &                ADAX, BDAX, CDAX, CAGEL
      DATA MCNT2, MCNT3/10, 10/
      POSMOT(C)= API*TEMP*C*(1.DO + BPI*C)**2
C  CHECK FOR REASONABLE INPUT VALUES.
      IF(CA1 .LT. 0.0 .OR. CA1 .GT. DENB) GO TO 10
      IF(CC1 .LT. 0.0 .OR. CC1 .GT. DENB) GO TO 10
      IF(V .LT. 0.0) GO TO 10
      GO TO 30
   10 CONTINUE
C  IF UNREALISTIC VALUES FROM GMSS ARE ENCOUNTERED, PRINT
C  AN ERROR MESSAGE AND DUMP THE MAJOR VARIABLES IN GETJ.
C  THEN RETURN.
      WRITE(6,20)CA1,CC1,V
   20 FORMAT(' IN GETJ ...UNREALISTIC INPUT VALUES.'/
     & ' CA1= ',G15.5,'    CC1= ',G15.5,'    V= ',G15.5)
       KGETJ= 1
      IF(JWRITE .LE. 0) JWRITE= 1
      GO TO 160
   30 CCNTINUE
C  CALCULATE BULK MASS FRACTIONS
          XA1= CA1/DENB
          XC1= CC1/DENB
C  CALCULATE REYNOLDS NUMBER
           RE= DF*V/VISC
        RE913= .0096*RE**.913
C  CALCULATE MASS TRANSFER COEFFICIENTS
          XXX= XA1*100.
          DDD= ADAX*XXX + BDAX*EXP(-CDAX*XXX)
          DAX= DDD*1.E-10
           SC= VISC/DAX
           SH= RE913*(SC**.346)
           KA= SH*DAX/DTUBE
           SC= VISC/DCX
           SH= RE913*(SC**.346)
           KC= SH*DCX/DTUBE
C  RESET KGETJ TO NON-ERROR CONDITION IF NEEDED.
      IF(KGETJ  .LE. 0) GO TO 40
       KGETJ= 0
   40 CONTINUE
```

```
C  USE INTERVAL HALVING TO FIND THE LARGEST POSSIBLE VALUE
C     OF CA2, REMEMBERING THAT (DELP - DELPI) MUST ALWAYS BE
C     POSITIVE.
      CA2BIG= DENB
      CA2SML= 0.
C  USE CA2 AS A TEMPORARY STORAGE LOCATION FOR NOW
         CA2= CA1 + CC1*RATIO
      PI2BIG= POSMOT(CA2) + DELP
      DO 60 I=1,20
         CA2= 0.5*(CA2BIG + CA2SML)
         PI2= POSMOT(CA2)
      IF(PI2 .GT. PI2BIG) GO TO 50
      CA2SML= CA2
      GO TO 60
   50 CA2BIG= CA2
   60 CONTINUE
C  SET UP LIMITS FOR OUTER LOOP TO FIND CA2
      CA2SML= CA1
      DO 130 I=1,MCNT2
         CA2= (CA2BIG + CA2SML)/2.
         JDA= KA*(CA2 - CA1)
C  SET UP LIMITS FOR INNER LOOP TO FIND CA3
      CA3BIG= CA1
      CA3SML= 0.
      DO 100 II=1,MCNT3
         CA3= 0.5D0*(CA3BIG + CA3SML)
         JB1= B*DENB*(CA2/CA3 - 1.0)
         CC2= (JB1*XC1 + KC*CC1)/
     &        (KC + C*(1. - DENB*C/(JB1 + DENB*C)))
         CC3= DENB*C*CC2/(JB1 + DENB*C)
        CEQ2= CA2 + CC2*RATIO
         PI2= POSMOT(CEQ2)
        CEQ3= CA3 + CC3*RATIO
         PI3= POSMOT(CEQ3)
       DELPI= PI2 - PI3
         JB2= GAMMA*(DELP - DELPI)
        CA3P= B*DENB*CA2/(JB2 + B*DENB)
      IF(JB2 .LT. 0.0) GO TO 70
      IF(CA3 .GT. CA3P) GO TO 80
   70 CA3SML= CA3
      GO TO 90
   80 CA3BIG= CA3
   90 CONTINUE
  100 CONTINUE
          JB= 0.5D0*(JB1 + JB2)
        CA2P= (JB*XA1 + KA*CA1 + B*CA3)/(KA + B)
      IF(CA2 .GT. CA2P) GO TO 110
      CA2SML= CA2
      GO TO 120
  110 CA2BIG= CA2
  120 CONTINUE
  130 CONTINUE
          JA= B*(CA2 - CA3)
          JC= C*(CC2 - CC3)
```

```
      IF(CAGEL .LT. 0.) GO TO 150
      IF(CA2 .LE. CAGEL) GO TO 150
         JDA= KA*(CAGEL - CA1)
          BX= JDA*(1. - B/KA)
          CX= BX*CAGEL*JDA
          JA= (-BX + DSQRT(BX*BX - 4.*CX))*0.5D0
          JB= (JA + JDA)/XA1
         CA3= DENB*JA/JB
          CX= C/(1. + DENB*C/JB)
       CCGEL= (JB*XC1 + KC*CC1)/(CX + KC)
          JC= CX*CCGEL
         JDC= KC*(CCGEL - CC1)
         CC3= DENB*JC/JB
        CEQ2= CAGEL + CCGEL*RATIO
         PI2= POSMOT(CEQ2)
        CEQ3= CA3 + CA3 + CC3*RATIO
         PI3= POSMOT(CEQ3)
       DELPI= PI2 - PI3
           Q= GAMMA*(DELP - DELPI)/JB
      IF(Q .LT. 1.) WRITE(6,140) Q
  140 FORMAT(' IN GETJ ... Q= ',G13.5,'  IS LESS THAN 1.')
  150 CONTINUE
  160 CONTINUE
C  THIS SECTION OF WRITE STATEMENTS PROVIDES A DUMP OF MAJOR
C    VARIABLES IN GETJ
      IF(JWRITE .LE. 0) GO TO 200
      JPRINT= JPRINT + 1
      IF(JPRINT .GE. JWRITE) JWRITE=  - 1000
      WRITE(6,170)JPRINT
  170 FORMAT(' ENTER GETJ ...PASS NUMBER ',I10)
      WRITE(6,190) CA1, CC1, V, DP, DENB
      WRITE(6,190) TEMP, MCNT2, MCNT3, VISC, DELP
      WRITE(6,190) JWRITE, JA, JB, JC
      WRITE(6,190) AKA, AKC, ERE, API, BPI
      WRITE(6,190) GAMMA, B, C, NP, RATIO
      WRITE(6,190) RE, KA, KC, DELPI
      WRITE(6,190) CA2, CC2, CEQ2, PI2
      WRITE(6,190) CA3, CC3, CEQ3, PI3
      WRITE(6,190) CA2SML, CA2BIG, CC2SML, CC2BIG
      WRITE(6,190) CA3SML, CA3BIG, CC3SML, CC3BIG
      WRITE(6,190) CCGEL, Q
      WRITE(6,180)
  180 FORMAT(1X,10('.'),' LEAVING GETJ  ',30('.'))
  190 FORMAT(5(1X,G15.5))
  200 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE RO
C
C  THIS IS THE FIBER REVERSE OSMOSIS INTERFACE
C
C                ________________
C       FEED    |                | PERMEATE
C      STREAM   |     FIBER      |-------------> 1
C   3 -------->|    REVERSE     | CONCENTRATE
C               |    OSMCSIS     |-------------> 2
C               |________________|
C
C  PARAMETER        QUANTITY
C      1            OPERATING PRESSURE
C      2            OPERATING TEMPERATURE
C      3            LENGTH OF A FIBER
C      4            OUTER RADIUS OF FIBER BUNDLE
C      5            INNER RADIUS OF FIBER BUNDLE
C      6            FIBER DIAMETER
C
C  THE PERMEATE STREAM MUST BE SPECIFIED FIRST
C  THE CONCENTRATE STREAM MUST BE STECIFIED SECOND
C  THE FEED STREAM MUST BE SPECIFIED THIRD
      REAL L,NF
      COMMON /LOOK/ ISW
      COMMON STREAM(4,100), ICONFG(8,100), PAR(500), NPAR,
     &       NCALL, IUNIT, NFATER, NS, NEQ, DESC(5)
      COMMON /ROFIT/  AKA, AKC, ERE, API, BPI, GAMMA, B, C,
     &                NF, RATIO
      COMMCN /PARMRO/ L, OR, RI, DF, TOLMX, TOLMN, NWRITE,
     &                NSTEPS
      COMMON /ROPARM/ TEMP, VISC, DELP, RHOB, MCNT2, MCNT3,
     &                JWRITE
      IF(NCALL) 10, 80, 90
   10 CONTINUE
C  SOME ERROR CHECKING
      IF(ICONFG(3,IUNIT) .LT. 0) GO TO 30
      WRITE(6,20) IUNIT, ICONFG(3,IUNIT)
   20 FORMAT(6X,'******ERROR, UNIT',I5,'. FIRST STREAM IN',
     &' CONFIGURATION IS',I5,', MUST BE PERMEATE (OUTPUT.)')
      NFATER= NFATER + 1
   30  IF(ICONFG(4,IUNIT) .LT. 0) GO TO 50
      WRITE(6,40) IUNIT, ICONFG(4,IUNIT)
   40 FORMAT(6X,'*****ERROR, UNIT',I5,'. SECOND STREAM IN',
     &'CONFIGURATION IS',I5,'.  MUST BE THE CONCENTRATE',
     & ' (OUTPUT).')
      NFATER= NFATER + 1
   50  IF(ICONFG(5,IUNIT) .GT. 0) GO TO 70
      WRITE(6,60) IUNIT, ICONFG(5,IUNIT)
   60 FORMAT(6X,'*****ERROR, UNIT',I5,'.  THIRD STREAM IN',
     &' CONFIGURATION IS',I5,'.  MUST BE THE FEED (INPUT).')
      NFATER= NFATER + 1
   70 CCNTINUE
      RETURN
```

```
   80 CONTINUE
C  INITIALIZATION IS THE SAME AS SIMULATE
C      RETURN
   90 CONTINUE
C  SIMULATE
        DELP= PAR(NPAR)
        TEMP= PAR(NPAR+1)
           L= PAR(NPAR+2)
          CR= PAR(NPAR+3)
          RI= PAR(NPAR+4)
          DF= PAR(NPAR+5)
       IPERM= -ICONFG(3,IUNIT)
       ICONC= -ICONFG(4,IUNIT)
       IFEED= ICONFG(5,IUNIT)
C  GET READY TO CALL ROSS
        FLOW= STREAM(1,IFEED)
         CAR= STREAM(3,IFEED)
      CARSAV= CAR
         CCR= STREAM(4,IFEED)
      CCRSAV= CCR
      CALL ROSS(FLOW,RHOB,CAR,CCR,SOUTA,SOUTB,SOUTC)
        TOUT= SOUTA + SOUTB + SOUTC
         XAP= SOUTA/TOUT
         XCP= SOUTC/TOUT
      STREAM(3,IPERM)= XAP*RHOB
      STREAM(4,IPERM)= XCP*RHOB
      STREAM(2,IPERM)= 0.
       FLOWC=FLOW-TOUT/RHOB
         CAC= (FLOW*CARSAV-SOUTA)/FLOWC
         CCC= (FLOW*CCRSAV-SOUTC)/FLOWC
      STREAM(3,ICONC)= CAC
      STREAM(4,ICONC)= CCC
C  NO SUSPENDED SOLIDS IN THE PERMEATE
      STREAM(2,ICONC)= FLOW*STREAM(2,IFEED)/FLOWC
      STREAM(1,ICONC)= FLOWC
      STREAM(1,IPERM)= FLOW - FLOWC
      IF(ISW.NE.0) WRITE(6,100)
  100 FORMAT('  LEAVING RO')
      IF(ISW.EQ.1) WRITE(6,110)IUNIT,(STREAM(I,IPERM),I=1,4)
     & (STREAM(I,ICONC),I=1,4)
  110 FORMAT(' UNIT',I5,' RO  PERM FLOW=',G10.3,5X,'SS=',
     &G10.3,5X,'DS=',G10.3,5X,'TOC=',G10.3/15X,'CONC FLOW=',
     & G10.3,5X,'SS=',G10.3,5X,'DS=',G10.5,'TOC=',G10.3)
      RETURN
      END
```

```
      SUBROUTINE ROSS(FLOW,RHOB,SCAR,SCCR,SOUTA,SOUTB,SOUTC)
C
C  THIS SUBROUTINE PERFORMS THE STEADY STATE RO CALCULATIONS
C
      REAL*8 R, JA, JB, JC, VR, DR, DRSAVE, CAR, CCR,
     &       OUTASV, OUTBSV, OUTCSV, ATOTAL, RDR, AUX,
     &       VRDR, CARDR, CCRDR, RELCA, RELCC, RELV,
     &       OUTA, OUTB, OUTC
      REAL NF,L
      EQUIVALENCE (IXCNT,IHALVE)
      COMMON /ROFIT/  AKA, AKC, ERE, API, BPI, GAMMA, B, C,
     &                NF, RATIO
      COMMON /FASTRO/ IFLAGF
      COMMON /PARMRO/ L, RO, RI, DF, TOLMX, TOLMN, NWRITE,
     &                NSTEPS
      DATA PI/3.141593/
      DATA IVFRST/0/
      DATA IERROR/0/
C  INITIALIZE COUNTERS
      IFLAGF= 0
      IF(IVFRST .NE. 0) GO TO 10
      IVFRST= 1
      IFLAGF= 1
   10 CONTINUE
         CAR= SCAR
         CCR= SCCR
      IHALVE= 0
           J= 0
           I= 0
        OUTA= 0.
        OUTB= 0.
        OUTC= 0.
           R= RI
      ATOTAL= PI*(RO*RO - RI*RI)
          VR= FLOW/(2.*PI*RI*L)
          DR= (RO - RI)/NSTEPS
      DRSAVE= DR
       KGETF= 10
   20 CONTINUE
C  START OF THE INTEGRATION LOOP
   30 CONTINUE
C  GETF CALCULATES VALUES OF THE FLUXES
      CALL GETF(CAR,CCR,VR,DF,JA,JB,JC,KGETF)
C  CHECK FOR ERRORS IN GETF
      IF(KGETF .EQ. 0) GO TO 100
      IERROR= IERROR + 1
      WRITE(6,40)
   40 FORMAT('  IN ROSS...RESPONDING TO AN ERROR IN GETF')
      WRITE(6,130) I, IXCNT, R, CAR, CCR, OUTA, OUTB, OUTC,
     &             VR, AUX, JA, JB, JC
       KGETF= 0
   50 CONTINUE
C  HALVE THE STEP SIZE
```

```
      IHALVE= IHALVE + 1
          DR= DR/2.
C  CHECK FOR EXCESSIVE STEP SIZE HALVINGS AND
C     ERRORS FROM GETF
      IF(IHALVE .LE. 20) GO TO 70
      WRITE(6,60)
   60 FORMAT(' IN ROSS. AN EXCESSIVE NUMBER OF RADIAL STEP'
     $,' SIZE HALVINGS HAVE OCCURRED.')
      STOP
   70 CONTINUE
      IF(IERROR .LE. 100) GO TO 90
      WRITE(6,80)
   80 FORMAT(' IN ROSS. AN EXCESSIVE NUMBER OF ERRORS HAVE'
     $,' BEEN REPORTED FROM GETF')
      STOP
   90 CONTINUE
  100 CONTINUE
C  ONE INTEGRATION STEP
         RDR= R + DR
         AUX= NF*DF*PI*DR*(2.*R+DR)
        VRDR= (2.*R*RHOB*VR-(JA+JB+JC)*AUX)/(2.*RDR*RHOB)
       CARDR= (2.*R*VR*CAR-JA*AUX)/(2.*RDR*VRDR)
       CCRDR= (2.*R*VR*CCR-JC*AUX)/(2.*RDR*VRDR)
C  CALCULATE THE RELATIVE CHANGE IN VARIABLES OVER THE
C    INTEGRATION STEP
      IF(VR .NE. 0.) RELV= (VRDR-VR)/VR
      IF(VR .EQ. 0.) RELV= VRDR-VR
      IF(CAR .NE. 0.) RELCA= (CARDR-CAR)/CAR
      IF(CAR .EQ. 0.) RELCA= CARDR-CAR
      IF(CCR .NE. 0.) RELCC= (CCRDR-CCR)/CCR
      IF(CCR .EQ. 0.) RELCC= CCRDR-CCR
C  CHECK FOR UNREALISTIC VALUES OF VARIABLES
      IF(VRDR .LT. 0.0) GO TO 50
      IF(CARDR .LT. 0.0) GO TO 50
      IF(CCRDR .LT. 0.0) GO TO 50
C  IF GRADIENTS ARE TOO STEEP, HALVE THE STEP SIZE
      IF(RELV .GT. TOLMX .OR. (-RELV).GT.TOLMX) GO TO 50
      IF(RELCA .GT. TOLMX .OR. (-RELCA).GT.TOLMX) GO TO 50
      IF(RELCC .GT. TOLMX .OR. (-RELCC).GT.TOLMX) GO TO 50
C  IF GRADIENTS ARE VERY SMALL, DOUBLE STEP SIZE
      IF(RELCA .GT. TOLMN .OR. (-RELCA) .GT. TOLMN) GO TO 11
      IF(RELCC .GT. TOLMN .OR. (-RELCC) .GT. TOLMN) GO TO 11
      IHALVE= IHALVE - 1
          DR= DR*2.
C  NEVER LET STEP SIZE BECOME LARGER THAN THE ORIGINAL ONE
      IF(DR.LT.DRSAVE ) GO TO 110
          DR= DRSAVE
      IHALVE= 0
  110 CONTINUE
C  UPDATA PERMEATE FLOW RATES
      OUTASV= OUTA
      OUTBSV= OUTB
      OUTCSV= OUTC
        OUTA= OUTA + JA*AUX*L*PI
```

```
         OUTB= OUTB + JB*AUX*L*PI
         OUTC= OUTC + JC*AUX*L*PI
C  GET READY FOR NEXT INTEGRATION STEP
            I= I + 1
            R= RDR
C  SAVE CURRENT VALUES OF VARIABLES FOR USE LATER
        VSAVE= VR
       CASAVE= CAR
       CCSAVE= CCR
           VR= VRDR
          CAR= CARDR
          CCR= CCRDR
C  DETERMINE WHETHER ANY OUTPUT AT THIS STEP IS REQUIRED
      IF(NWRITE .LE. 0) GO TO 140
           J= J + 1
      IF(J.LT.NWRITE) GO TO 140
           J= 0
  120 CONTINUE
      WRITE(6,130) I, IXCNT, R, CAR, CCR, OUTA, OUTB, OUTC,
     &             VR, AUX, JA, JB, JC
  130 FORMAT(' IN ROSS ',2I3,(/5(1X,E11.4)))
      IF(R .EQ. RO) GO TO 150
  140 CONTINUE
      IF(R .LT. RO-DR/10.) GO TO 20
C  USE LINEAR INTERPOLATION TO FIND VALUES OF CAR,CCR,VR
C    EXACTLY AT RO
          VR= ((VRDR-VSAVE)/DR)*(RO-(RDR-DR)) + VSAVE
         CAR= ((CARDR-CASAVE)/DR)*(RO-(RDR-DR)) + CASAVE
         CCR= ((CCRDR-CCSAVE)/DR)*(RO-(RDR-DR)) + CCSAVE
        OUTA= ((OUTA-OUTASV)/DR)*(RO-(RDR-DR)) + OUTASV
        OUTB= ((OUTB-OUTBSV)/DR)*(RO-(RDR-DR)) + OUTBSV
        OUTC= ((OUTC-OUTCSV)/DR)*(RO-(RDR-DR)) + OUTCSV
           R= RO
      IF(NWRITE .EQ. -999 .OR. NWRITE .GT. 0) GO TO 120
  150 CONTINUE
C  UNSAVE THE ORIGINAL STEP SIZE
          DR= DRSAVE
       SOUTA= OUTA
       SOUTB= OUTB
       SOUTC= OUTC
        SCAR= CAR
        SCCR= CCR
      RETURN
      END
```

```
      SUBROUTINE GETF(CA1,CC1,V,DF,JA,JB,JC,KGETF)
C
C  THIS SUBROUTINE CCMPUTES THE FLUXES FOR THE
C  REVERSE OSMOSIS PROGRAM
C  SEE REPORT BY SMITH AND STARKS ON THE RO UNIT FOR A
C    DISCRIPTICN OF VARIABLES
C
      REAL*8 JA, JB, JC, CA1, CC1, V, XA1, XC1, CA2BIG,
     &       CA2SML, PI2BIG, PI, POSMOT, CA2, JDA, CA3BIG,
     &       CA3SML, CA3, JB1, CC2, CC3, CEQ2, PI2, CEQ3,
     &       PI3, DELPI, JB2, CA3P, CA2P, CONC
      REAL KA,KC,NF
      COMMCN /ROPARM/ TEMP, VISC, DELP, RHO, MCNT2, MCNT3,
     &                JWRITE
      COMMON /ROFIT/  AKA, AKC, ERE, API, BPI, GAMMA, B, C,
     &                NF, RATIO
      COMMCN /FASTRO/ IFLAG
      DATA TOLER/0.001/
      DATA JPRINT/0/
      POSMCT(CONC)= API*TEMP*CONC*(1.0+BPI*CONC)**2
      IF(CA1 .LT. 0.0 .OR. CA1 .GT. RHO) GO TO 10
      IF(CC1 .LT. 0.0 .OR. CC1 .GT. RHO) GO TO 10
      IF(V .LT. 0.0) GO TO 10
      GO TO 30
   10 CONTINUE
C  IF UNREALISTIC VALUES FROM ROSS ARE ENCOUNTERED, PRINT
C  AN ERROR MESSAGE AND DUMP THE MAJOR VARIABLES IN GETF.
C  THEN RETURN.
      WRITE(6,20) CA1,CC1,V
   20 FORMAT(' IN GETF ...UNREALISTIC INPUT VALUES.',
     & ' CA1= ',G15.5,'     CC1= ',G15.5,'     V= ',G15.5)
       KGETF= 1
      IF(JWRITE .LE. 0) JWRITE= 1
      GO TO 140
   30 CONTINUE
C  CALCULATE REYNOLDS NUMBER
          RE= DF*V/VISC
C  CALCULATE MASS TRANSFER COEFFICIENTS
          KA= AKA*RE**ERE
          KC= AKC*RE**ERE
C  RESET KGETF TO NON-ERROR CONDITION IF NEEDED.
      IF(KGETF .LE. 0) GO TO 40
       KGETF= 0
   40 CONTINUE
C  CALCULATE BULK MASS FRACTIONS
         XA1= CA1/RHO
         XC1= CC1/RHO
      IF(IFLAG .EQ. 0) GO TO 190
C  USE INTERVAL HALVING TO FIND THE LARGEST POSSIBLE VALUE
C    OF CA2, REMEMBERING THAT (DELP-DELPI) MUST ALWAYS BE
C    POSITIVE.
      CA2BIG= RHO
      CA2SML= 0.
```

```
C  USE CA2 AS A TEMPORARY STORAGE LOCATION FOR NOW
         CA2= CA1 + CC1*RATIO
      PI2BIG= POSMOT(CA2) + DELP
      DO 60 I= 1,20
         CA2= (CA2BIG + CA2SML)/2.
         PI2= POSMOT(CA2)
      IF(PI2 .GT. PI2BIG) GO TO 50
      CA2SML= CA2
      GO TO 60
   50 CA2BIG= CA2
   60 CONTINUE
C  USE DOUBLLY NESTED INTERVAL HALVING TO SOLVE FOR
C     CA2 AND CA3
C  SET UP LIMITS FOR OUTER LOOP TO FIND CA2
      CA2SML= CA1
      CA2BIG= CA2
      DO 130 I= 1,MCNT2
         CA2= (CA2BIG + CA2SML)/2.
         JDA= KA*(CA2 - CA1)
C  SET UP LIMITS FOR INNER LOOP TO FIND CA3
      CA3BIG= CA1
      CA3SML= 0.
      DO 100 II= 1,MCNT3
         CA3= (CA3BIG + CA3SML)/2.
         JB1= B*RHO*(CA2/CA3 - 1.0)
         CC2= (JB1*XC1+KC*CC1)/(KC+C*(1.-RHO*C/(JB1+RHO*C)))
         CC3= RHO*C*CC2/(JB1+RHO*C)
        CEQ2= CA2 + CC2*RATIO
         PI2= POSMOT(CEQ2)
        CEQ3= CA3 + CC3*RATIO
         PI3= POSMOT(CEQ3)
       DELPI= PI2 - PI3
         JB2= GAMMA*(DELP - DELPI)
        CA3P= B*RHO*CA2/(JB2 + B*RHO)
      IF(JB2 .LT. 0.0) GO TO 70
      IF(CA3 .GT. CA3P) GO TO 80
   70 CA3SML= CA3
      GO TO 90
   80 CA3BIG= CA3
   90 CONTINUE
  100 CONTINUE
          JB= (JB1 + JB2)/2.
        CA2P= (JB*XA1 + KA*CA1 + B*CA3)/(KA + B)
      IF(CA2 .GT. CA2P) GO TO 110
      CA2SML= CA2
      GO TO 120
  110 CA2BIG= CA2
  120 CONTINUE
  130 CONTINUE
          JA= B*(CA2 - CA3)
          JC= C*(CC2 - CC3)
  140 CONTINUE
C  THIS SECTION OF WRITE STATEMENTS PROVIDES A DUMP OF MAJOR
C     VARIABLES IN GETF
```

```
      IF(JWRITE .LE. 0) GO TO 180
      JPRINT= JPRINT + 1
      IF(JPRINT .GE. JWRITE) JWRITE=-1000
      WRITE(6,150) JPRINT
  150 FORMAT(' ENTER GETF ...PASS NUMBER ',I10)
      WRITE(6,170) CA1, CC1, V, DF, RHO
      WRITE(6,170) TEMP, MCNT2, MCNT3, VISC, DELP
      WRITE(6,170) JWRITE, JA, JB, JC
      WRITE(6,170) AKA, AKC, ERE, API, BPI
      WRITE(6,170) GAMMA, B, C, NF, RATIO
      WRITE(6,170) RE, KA, KC, DELPI
      WRITE(6,170) CA2, CC2, CEQ2, PI2
      WRITE(6,170) CA3, CC3, CEQ3, PI3
      WRITE(6,170) CA2SML, CA2BIG, CC2SML, CC2BIG
      WRITE(6,170) CA3SML, CA3BIG, CC3SML, CC3BIG
      WRITE(6,160)
  160 FORMAT(1X,10('.'),' LEAVING GETF  ',30('.'))
  170 FORMAT(5(1X,G15.5))
  180 CONTINUE
      RETURN
  190 CONTINUE
C  TRY BACK SUBSTITUTION
      DO 200 I=1,15
        CA2L= CA2
        CA3L= CA3
        CC2L= CC2
        CC3L= CC3
        CEQ2= CA2 + RATIO*CC2
         PI2= POSMOT(CEQ2)
        CEQ3= CA3 + RATIO*CC3
         PI3= POSMOT(CEQ3)
       DELPI= PI2 - PI3
      IF(DELPI .GT. DELP) DELPI= 0.3*DELP
          JB= GAMMA*(DELP-DELPI)
          JA= B*(CA2-CA3)
          JC= C*(CC2-CC3)
       TOTLJ= JA+JC+JB
         CA3= JA/TOTLJ
         CC3= JC/TOTLJ
         CA2= (TOTLJ*XA1+KA*CA1+B*CA3)/(KA+B)
         CC2= (TOTLJ*XC1+KC*CC1+C*CC3)/(KC+C)
      RELCA3= (CA3-CA3L)/CA3
      RELCC3= (CC3-CC3L)/CC3
      RELCA2= (CA2-CA2L)/CA2
      RELCC2= (CC2-CC2L)/CC2
      IF(RELCA3 .LT. 0.) RELCA3= -RELCA3
      IF(RELCC3 .LT. 0.) RELCC3= -RELCC3
      IF(RELCA2 .LT. 0.) RELCA2= -RELCA2
      IF(RELCC2 .LT. 0.) RELCC2= -RELCC2
      IF(RELCA3 .GT. TOLER) GO TO 200
      IF(RELCC3 .GT. TOLER) GO TO 200
      IF(RELCC2 .GT. TOLER) GO TO 200
      IF(RELCA2 .GT. TOLER) GO TO 200
      GO TO 140
```

```
200 CONTINUE
      IFLAG= 1
     GO TO 30
     END
```

```
      SUBROUTINE TR
C
C  TUBULAR REVERSE OSMOSIS MODEL INTERFACE TO WPE SIMULATOR
C
C                     ---------------
C                    |               | PERMEATE
C          FEED      |    TUBULAR    |------------> 1
C       3 -------->  |    REVERSE    | CONCENTRATE
C                    |    OSMOSIS    |------------> 2
C                    |_______________|
C
C  PARAMETER         QUANTITY
C       1            NUMBER OF TUBES
C       2            OPERATING TEMPERATURE
C       3            PRESSURE DROP ACROSS THE MEMBRANE
C                    AT THE INLET
C       4            PRESSURE DROP DOWN THE TUBE
C       5            DIAMETER OF TUBE
C       6            TUBE LENGTH
C
C  THE PERMEATE STREAM MUST BE SPECIFIED FIRST
C  THE CONCENTRATE STREAM MUST BE SPECIFIED SECOND
C  THE FEED STREAM MUST BE SPECIFIED THIRD
      REAL NTPIDT
      DIMENSION PERMN(100)
      COMMON /LOOK/ ISW
      COMMON STREAM(4,100), ICONFG(8,100), PAR(500), NPAR,
     &       NCALL, IUNIT, NFATER, NS, NEQ, DESC(5)
      COMMON /TRPARM/ PLEN, DTUBE, NT, JPRINT, JWRITE
      COMMON /PARMTR/ TEMP, VISC, DENB, DPZERO, PDROP
      IF(NCALL) 10, 80, 90
C THERE ARE NO MATERIAL BALANCE CALCULATIONS.  HOWEVER, THE
C  STREAM SPECIFICATIONS ARE CHECKED FOR CONSISTENT
C   INPUT/OUTPUT
   10 CONTINUE
C  SOME ERROR CHECKING
      IF(ICONFG(3,IUNIT) .LT. 0) GO TO 30
      WRITE(6,20) IUNIT, ICONFG(3,IUNIT)
   20 FORMAT(6X,'*****ERROR, UNIT',I5,'.  FIRST STREAM IN',
     & ' CONFIGURATION IS',I5,'. MUST BE THE PERMEATE',
     & ' (OUTPUT).')
      NFATER= NFATER + 1
   30 IF(ICONFG(4,IUNIT) .LT. 0) GO TO 50
      WRITE(6,40) IUNIT, ICONFG(4,IUNIT)
   40 FORMAT(6X,'*****ERROR, UNIT',I5,'.  SECOND STREAM IN',
     & ' CONFIGURATION IS',I5,'. MUST BE THE CONCENTRATE',
     & ' (OUTPUT).')
      NFATER= NFATER + 1
   50 IF(ICONFG(5,IUNIT) .GT. 0) GO TO 70
      WRITE(6,60) IUNIT, ICONFG(5,IUNIT)
   60 FORMAT(6X,'*****ERROR, UNIT',I5,'.  THIRD STREAM IN',
     & ' CONFIGURATION IS',I5,'. MUST BE THE FEED (INPUT).')
      NFATER= NFATER + 1
```

```
   70 CONTINUE
      RETURN
   80 CCNTINUE
C  INITIALIZATION SAME AS SIMULATE
      PERMN(IUNIT) = C.
C     RETURN
   90 CONTINUE
C  SET UP COMMON VARIABLES
          NT= PAR(NPAR)
        TEMP= PAR(NPAR+1)
      DPZERO= PAR(NPAR+2)
       PDROP= PAR(NPAR+3)
       DTUBE= PAR(NPAR+4)
        PLEN= PAR(NPAR+5)
C  SIMULATE
       IPERM= -ICONFG(3,IUNIT)
       ICONC= -ICONFG(4,IUNIT)
       IFEED= ICONFG(5,IUNIT)
C  GET READY TO CALL TRSS
      KULTRA= -1
          CS= STREAM(2,IFEED)
          CD= STREAM(3,IFEED)
          CC= STREAM(4,IFEED)
        FLOW= STREAM(1,IFEED)
        PERM= PERMN(IUNIT)
      IF(ISW .GE. 1)
     & WRITE(6,100) IPERM, ICONC, IFEED, CA, CC, FLOW
  100 FORMAT(' $$$ TR DEBUG',6G10.3)
      CALL TRSS(KULTRA,CS,CD,CC,FLOW,TOTALA,TOTALB,
     &          TOTALC,PERM)
         PERMN(IUNIT) = PERM
               TOTAL= TOTALA + TOTALB + TOTALC
      STREAM(3,IPERM) = TOTALA/TOTAL*DENB
      STREAM(4,IPERM) = TOTALC/TOTAL*DENB
      STREAM(1,IPERM)= TOTAL/DENB
C NO SUSPENDED SOLIDS PASS THROUGH TR MEMBRANE
      STREAM(2,IPERM) = 0.
C  CHECK FOR ERRORS
      IF(KULTRA .LT. 0) GO TO 120
      WRITE(6,110) KULTRA
  110 FORMAT(' *****ERROR IN TR WHILE CALLING TRSS.',
     & ' KULTRA=',I5)
      NFATER= NFATER + 1
  120 CONTINUE
C  GET FLOW RATE OF CONC. BY STEADY STATE MATERIAL BALANCE
      STREAM(1,ICONC) = STREAM(1,IFEED)-STREAM(1,IPERM)
C  GET CONCENTRATICN OF CONCENTRATE BY COMPONENT BALANCE
      DO 130 I=2,4
      STREAM(I,ICONC) = (STREAM(I,IFEED)*STREAM(1,IFEED)-
     &   STREAM(I,IPERM)*STREAM(1,IPERM))/STREAM(1,ICONC)
  130    CONTINUE
      IF(ISW.EQ.1) WRITE(6,140)IUNIT,(STREAM(I,IPERM),I=1,4)
     & (STREAM(I,ICONC),I=1,4)
  140 FORMAT(' UNIT',I5,' TR  PERM FLOW=',G10.3,5X,'SS=',
```

```
&G10.3,5X,'DS=',G10.3,5X,'TOC=',G10.3/15X,'CONC FLOW=',
& G10.3,5X,'SS=',G10.3,5X,'DS=',G10.3,5X,'TOC=',G10.3)
 RETURN
 END
```

```
      SUBROUTINE TRSS(KULTRA,SS,DS,TC,F,TOTALA,TOTALB,
     &                TOTALC,PERM)
C
C  THIS SUBROUTINE PERFORMS THE STEADY STATE CALCULATIONS
C    FOR TUBULAR REVERSE OSMOSIS MODULES.
C  THIS ROUTINE ASSUMES COMPLETE REJECTION OF SUSPENDED
C    SOLIDS AND HIGH REJECTION OF DESOLVED SOLIDS.
C  SEE THE REPORT BY ABBOTT AND STERLING ON THE MODIFIED UF/
C    TUBULAR RO/ GEL MODEL FOR A DISCRIPTION OF VARIABLES
C
      REAL NTPIDT
      REAL*8 RE, SCA, SHA, KA, SCC, SHC, KC
      COMMON /TRPARM/ PLEN, DTUBE, NT, JPRINT, JWRITE
      COMMON /TRFIT/  GAM1, GAM2, GAMINF, API, B, C, DCX,
     &                ADAX, BDAX, CDAX
      COMMON /PARMTR/ TEMP, VISC, DENB, DPZERO, PDROP
      COMMON /CTIME/  TIME, FTIME, DT
      DATA PIE/3.141593/
C  COMPUTE NT TIMES THE CIRCUMFERENCE OF ALL TUBES
      NTPIDT= NT*DTUBE*PIE
C  COMPUTE THE CROSS-SECTIONAL AREA OF A TUBE
        AREA= PIE*DTUBE*DTUBE/4.
C  COMPUTE THE VELOCITY THROUGH A TUBE
           V= F/(AREA*NT)
          CA= DS
C  COMPUTE THE WEIGHT FRACTION OF TDS
         XA1= DS/DENB
C  COMPUTE THE WEIGHT FRACTION OF TOC
         XC1= TC/DENB
C  COMPUTE THE REYNOLDS NUMBER
          RE= DTUBE*V/VISC
       RE913= 0.0096*RE**.913
         XXX= XA1*100.
      DD= ADAX*XXX
      IF(CDAX*XXX .LT. 174.) DDD= ADAX*XXX + BDAX*EXP(-CDAX*
         DAX= DDD*1.E-10
      IF(DAX .NE. 0.) GO TO 10
      KULTRA= 1
      GO TO 100
   10    SCA= VISC/DAX
      IF(SCA .GT. 0.) GO TO 20
      KULTRA= 2
      GO TO 100
   20    SHA= RE913*(SCA**.346)
          KA= SHA*DAX/DTUBE
      IF(DCX .NE. 0.) GO TO 30
      KULTRA= 3
      GO TO 100
   30    SCC= VISC/DCX
      IF(SCC .GT. 0.) GO TO 40
      KULTRA= 4
      GO TO 100
   40    SHC= RE913*(SCC**.346)
```

```
        KC= SHC*DCX/DTUBE
     DPBAR= DPZERO - 0.5*PDROP
       POS= API*TEMP*CA
    IF(POS .LE. DPBAR) GO TO 50
    KULTRA= 5
    GO TO 100
 50  GAMMA= GAMINF
    IF(GAM2*PERM .LT. 174)
   & GAMMA= GAMINF + (GAM1 - GAMINF)*EXP(-GAM2*PERM)
     TERM1= GAMMA*DPBAR/DENB + KA
     TERM2= GAMMA*POS/DENB + B + KA
    IF(TERM2 .NE. 0.) GO TO 60
    KULTRA= 6
    GO TO 100
 60 TERM12= TERM1/TERM2
    TOTALB= PLEN*GAMMA*(DPBAR - POS*TERM12)*NTPIDT
      PERM= PERM + (TOTALB/DENB)*DT
    TOTALA= B*DS*PLEN*TERM12*NTPIDT
    TOTALC= C*TC/(C + KC)*(KC*PLEN*NTPIDT + TOTALB/DENB)
    IF(TOTALA .LT. 0.) WRITE(6,70) TOTALA, B, TERM12
 70 FORMAT(' *****TOTALA= ',G12.5,'   B= ',G12.5,
   &      '   TERM12= ',G12.5)
    IF(TOTALB .LT. 0.) WRITE(6,80) TOTALB,GAMMA,POS,TERM12
 80 FORMAT(' *****TOTALB= ',G12.5,'   GAMMA= ',G12.5,
   & '   POS= ',G12.5,'   TERM12= ',G12.5)
    IF(TOTALC .LT. 0.) WRITE(6,90) TOTALC,C,KC
 90 FORMAT(' *****TOTALC= ',G12.5,'   C= ',G12.5,
   & '   KC= ',G12.5)
100 IF(JPRINT .LE. 0) RETURN
    JPRINT= JPRINT - 1
    WRITE(6,110) SS, DS, TC, F, DPZERO, PDROP, PLEN, DT,
   &            DTUBE, NTPIDT, DENB, NT
110 FORMAT('      SS=',G13.5,'      DS=',G13.5,'      TC=',
   * G13.5,'       F=',G13.5/' DPZERO=',G12.5,'  PDROP=',
   1 G13.5,'    PLEN=',G13.5,'      DT=',G13.5/'  DTUBE=',
   2 G13.5,' NTPIDT=',G13.5,'    DENB=',G13.5,'      NT=',
   3 G13.5)
    WRITE(6,120) GAM1, GAM2, GAMINF, API, B, C, DCX, ADAX,
   &            BDAX, CDAX
120 FORMAT('    GAM1=',G13.5,'    GAM2=',G13.5,' GAMINF=',
   * G13.5,'       B=',G13.5,'       C=',G13.5/'  RATIO=',
   1 G13.5,'     DCX=',G13.5,'    ADAX=',G13.5,'   BDAX=',
   2 G13.5,'    CDAX=',G13.5)
    WRITE(6,130) TEMP, VISC, AREA, V, CA, XA1, XC1, RE
130 FORMAT('    TEMP=',G13.5,'    VISC=',G13.5,'   AREA=',
   * G13.5,'       V=',G13.5/'      CA=',G13.5,'    XA1=',
   1 G13.5,'     XC1=',G13.5,'      RE=',G13.5)
    WRITE(6,140) DAX, SCA, SHA, KA, DCX, SCC, SHC, KC
140 FORMAT('     DAX=',G13.5,'     SCA=',G13.5,'     SHA=',
   * G13.5,'      KA=',G13.5/'     DCX=',G13.5,'     SCC=',
   1 G13.5,'     SHC=',G13.5,'      KC=',G13.5)
    WRITE(6,150) DPBAR, POS, TERM1, TERM2, TERM12,
   &            TOTALA, TOTALB, TOTALC
150 FORMAT('  DPBAR=',G13.5,'     POS=',G13.5,'  TERM1=',
```

```
     1 G13.5,'  TERM2=',G13.5/' TERM12=',G13.5,' TOTALA=',
     2 G13.5,' TOTALB=',G13.5,' TOTALC=',G13.5)
 160 RETURN
     END
```

```
      SUBRCUTINE UV
C
C  THIS IS THE ULTRAVIOLET OZONATION INTERFACE
C
C                      ________________   PURGE
C         FEED        |                |---------->
C     1 --------->|  ULTRAVIOLET   |
C                 |   OZONATION    |  EFFLUENT
C         OZONE   |                |----------> 2
C       --------->|________________|
C
C  PARAMETER        QUANTITY
C      1            INITIAL TSS CONC.
C      2            INITIAL TDS CONC.
C      3            INITIAL TOC CONC.
C      4            INLET GAS PHASE OZONE TO AIR MASS RATIO
C      5            VOLUMETRIC GAS FLOW RATE
C      6            PRECONTACTOR FLAG (0= NO PRECONTACTOR)
C      7            NUMBER OF STAGES
C      8            AREA OF A CONTACTOR
C      9            AREA OF THE PRECONTACTOR
C     10            HEIGHT OF A STAGE
C     11            FEED TEMPERATURE
C     12            OPERATING PRESSURE
C  THE FEED STREAM MUST BE SPECIFIED FIRST
C  THE EFFLUENT STREAM MUST BE SPECIFIED SECOND
      DIMENSION ZOUT(10), CZOUT(10), CTOUT(10), SS(10),
     &          DS(10), DSS(10), DDS(10)
      COMMON /DELTAT/ DTUV
      COMMON /MATTOC/ TOCRCT
      COMMON /MATBAL/ BALNCE(4), AMTIN(4), AMTOUT(4)
      COMMON /CTIME/  TIME, FTIME, DT
      COMMON STREAM(4,100), ICONFG(8,100), PAR(500), NPAR,
     &       NCALL, IUNIT, NFATER, NS, NEQ, DESC(5)
      COMMON /LOOK/   ISW
      COMMON /STAGES/ NSTAGE, PRECON
      COMMON /MATDIS/ MATCAL
      COMMON /UVPARM/ CAREA, PAREA, H, RHO, PRESS, TEMP, NWR
      COMMON /STGSAV/ ZOUT, CZOUT, CTOUT, SS, DS
      IF(NCALL) 10, 100, 110
   10 CONTINUE
C  INITILIZE
      PRECON= PAR(NPAR+5)
      NSTAGE= PAR(NPAR+6)
         NNN= NSTAGE
      IF(PRECON .NE. 0.0) NNN= NSTAGE + 1
      IF(MATCAL .NE. 0) GO TO 30
      DO 20 I= 1, NNN
      CZOUT(I)= 0.
       ZOUT(I)= 0.
         SS(I)= PAR(NPAR)
         DS(I)= PAR(NPAR+1)
   20 CTOUT(I)= PAR(NPAR+2)
```

```
   30 CCNTINUE
           FLAG= 0.
        IF(PRECON .NE. 0.0) FLAG=1.
           VCON= CAREA*H
           VPRE= PAREA*H
        BALNCE(1)= BALNCE(1)  + NSTAGE*VCON+FLAG*VPRE
        DC 40 I= 1, NSTAGE
        BALNCE(2)= BALNCE(2)  + VCON*SS(I)
        BALNCE(3)= BALNCE(3)  + VCON*DS(I)
        BALNCE(4)= BALNCE(4)  + VCON*CTOUT(I)
   40 CONTINUE
        IF(PRECON .EQ. 0.0) GO TC 50
        BALNCE(2)= BALNCE(2)  + VPRE*SS(NSTAGE+1)
        BALNCE(3)= BALNCE(3)  + VPRE*DS(NSTAGE+1)
        BALNCE(4)= BALNCE(4)  + VPRE*CTOUT(NSTAGE+1)
   50 CONTINUE
        IF(ICONFG(3,IUNIT) .GT. 0) GO TO 70
        WRITE(6,60) IUNIT, ICONFG(3,IUNIT)
   60 FORMAT(6X,'****ERROR, UNIT',I5,'.  FIRST STREAM IN',
       &  ' CONFIGURATICN IS',I5,'.  MUST BE THE FEED.')
        NFATER= NFATER + 1
   70 IF(ICONFG(4,IUNIT) .LT. 0) GO TO 90
        WRITE(6,80) IUNIT, ICONFG(4,IUNIT)
   80 FORMAT(6X,'****ERROR, UNIT',I5,'. SECOND STREAM IN',
       &  ' CONFIGURATION IS',I5,'.  MUST BE THE EFFLUENT.')
        NFATER= NFATER + 1
   90 CCNTINUE
  100 CONTINUE
        RETURN
  110 CONTINUE
          DTUV= DT
C  ALL COMMON VARIABLES ARE ALREADY SET UP
C  BEGIN SIMULATION
         IFEED= ICONFG(3,IUNIT)
         IPROD= -ICONFG(4,IUNIT)
          CZIN= 0.0
          CTIN= STREAM(4,IFEED)
           ZIN= PAR(NPAR+3)
             G= PAR(NPAR+4)/NSTAGE
         CAREA= PAR(NPAR+7)
         PAREA= PAR(NPAR+8)
             H= PAR(NPAR+9)
          TEMP= PAR(NPAR+10)
         PRESS= PAR(NPAR+11)
             F= STREAM(1,IFEED)
        IF(ISW .GT. 1) WRITE(6,120) F, CTIN
  120 FORMAT('OUV...BEFORE CALL TO UOZONE,FLOW=',G10.3,
       &  '          TOC CONC.=',G10.3)
        TOCRCT= 0.
        CALL UOZONE(ZIN,CZIN,CTIN,G,F,ZOUT,CZOUT,CTOUT)
C  DETERMINE IF PRE-CONTACTOR IS PRESENT
            NNN= NSTAGE
        IF(PRECON .NE. 0.0) NNN= NSTAGE + 1
        STREAM(4,IPROD)= CTOUT(NSTAGE)
```

```
      STREAM(1,IPROD)=  F
            AMTOUT(4)= AMTOUT(4)  + TOCRCT
      IF(ISW .GT. 1 )WRITE(6,130) F, CTOUT(NSTAGE)
 130  FORMAT(' UV...AFTER CALL TO UOZONE, FLOW=',G10.3,
     &        5X,'TOC CONC.=',G10.3)
        VPRE= PAREA*H
        VCON= CAREA*H
      DO 160 I= 1 ,NNN
      IF(I .EQ. 1) GO TO 140
         VCL= VCON
         SSO= SS(I-1)
         DSO= DS(I-1)
      GO TO 150
 140  CONTINUE
         VOL= VPRE
         SSO= STREAM(2,IFFED)
         DSO= STREAM(3,IFEED)
 150  CONTINUE
      DDS(I)= F*(DSO-DS(I))/VOL
      DSS(I)= F*(SSO-SS(I))/VOL
 160  CONTINUE
      DO 170 I= 1, NNN
       SS(I)= SS(I)  + DSS(I)*DT
       DS(I)= DS(I)  + DDS(I)*DT
 170  CONTINUE
      STREAM(2,IPROD)= SS(NNN)
      STREAM(3,IPROD)= DS(NNN)
      IF(ISW .EQ. 1)
     & WRITE(6,180)  (SS(I),I=1,NNN),(DS(I),I=1,NNN)
 180  FORMAT(' UV',I10,8G10.3,/I10,8G10.3)
      RETURN
      END
```

```
      SUBROUTINE UOZONE(ZINO,CZINO,TOCINO,G,F,ZOUT,CZOUT,
     &                  TOCOUT)
C
C  THIS SUBROUTINE PERFORMS THE STEADY STATE CALCULATIOS
C  FOR  THE ULTRAVIOLET OZONATION UNIT
C
      REAL KLA, KHENRY, KRATE, KDCOMP
      COMMON /DELTAT/ DT
      COMMON /UVL/    UVLITE
      COMMON /OPIT/   KHENRY, ECOZ, ETOC, KRATE, KDCOMP,
     &                EOZD, UVEFCT, ALPHA, EN, QPRIME
      COMMON /OZOPER/ CAREA, PAREA, H, RHO, PRESS, TEMP, NWR
      DIMENSION ZOUT(10), CZOUT(10), TOCOUT(10), DCZBR(10),
     &          DTOCBR(10)
      COMMON /STAGES/ NSTAGE,PRECON
      DATA IFIRST/0/
      EQUIVALENCE (NNN,IEND)
         NNN= NSTAGE
      IF(PRECON .NE. 0.0) NNN= NSTAGE + 1
      IF(IFIRST .NE. 0) GO TO 20
C  FOR FIRST ITERATION, SET UP INLET GAS CONCENTRATION
C   TO PRE-CONTACTOR
      IFIRST= 1
       TZOUT= 0.
      DO 10 I= 1, NSTAGE
   10  TZOUT= TZOUT + ZOUT(I)
        ZBAR= TZOUT/NSTAGE
   20 CONTINUE
      UVLITE= 0.
C CALL FOR PRE-CONTACTOR
      CALL USTAGE(ZBAR, CZINO, TOCINO, NSTAGE*G, F,
     & ZOUT(NSTAGE+1), DCZBR(NSTAGE+1), DTOCBR(NSTAGE+1),
     & PAREA, CZOUT(NSTAGE+1), TOCOUT(NSTAGE+1))
       TZOUT= 0.
C SET UP UV RADIATION EFFECT ON REACTION RATE CONSTANTS
      UVLITE= UVEFCT
      DO 60 I= 1, NSTAGE
C SET UP INPUTS TO THE NEXT STAGE
         ZIN= ZINO
           N= I - 1
      IF(I .NE. 1) GO TO 30
           N= NSTAGE + 1
      IF(PRECON .EQ. 0.0) GO TO 40
   30 CONTINUE
        CZIN= CZOUT(N)
       TOCIN= TOCOUT(N)
      GO TO 50
   40 CONTINUE
        CZIN= CZINO
       TOCIN= TOCINO
   50 CONTINUE
      CALL USTAGE(ZIN, CZIN, TOCIN, G, F, ZOUT(I), DCZBR(I),
     & DTOCBR(I), CAREA, CZOUT(I), TOCOUT(I))
```

```
      TZOUT= TZOUT + ZOUT(I)
   60 CONTINUE
C DETERMINE NEXT GAS CONCENTRATION TO THE PRE-CONTACTOR
       ZBAR= TZOUT/NSTAGE
      DO 70 I= 1, IEND
C TAKE ONE INTEGRATION STEP
      CZOUT(I) = CZOUT(I)  + DCZBR(I)*DT
   70 TOCOUT(I)= TOCOUT(I)  + DTOCBR(I)*DT
      RETURN
      END
```

```
      SUBROUTINE USTAGE(ZIN,CZIN,TOCIN,G,F,ZOUT,DCZ,DTOC,
     &                  AREA,CZOUT,TOCOUT)
C
C  THIS SUBROUTINE PERFORMS THE STEADY STATE CALCULATIONS
C   FOR A SINGLE UV STAGE
C
      REAL KLA, KHENRY, KRATE, KDCOMP
      EQUIVALENCE (DCOMP,DECOMP), (NSTWRT,NWRITE)
      COMMON /DELTAT/ DT
      COMMON /MATTOC/ TOCRCT
      COMMON /UVFIT/  KHENRY, ECOZ, ETOC, KRATE, KDCOMP,
     &                EOZD, UVEFCT, ALPHA, EN, QPRIME
      COMMON /UVL/    UVLITE
      COMMON /UVPARM/ CAREA, PAREA, H, RHO, PRESS, TEMP,
     &                NWRITE
      COMMON /GASLAW/ RGAS
      DATA JWRITE /0/
C USE IDEAL GAS LAW FOR DETERMINING GAS DENSITY
      RHOGAS= PRESS/TEMP/RGAS
           V= AREA*H
          CZ= CZOUT
         TOC= TOCOUT
C DETERMINE LIQUID PHASE RESIDENCE TIME
         TAU= V/F
         YIN= ZIN/(1.0+ZIN)
      GMOLES= G*RHOGAS*(1.-YIN)
         AUX= RHO/KHENRY
C DETERMINE M1(H)
         XYZ= EXP(-RHO*QPRIME*AREA*G**(1.-EN)/
     &                 (KHENRY*V*RHOGAS))
C SET UP REACTION RATE CONSTANTS
        RATE= KRATE*(1. + UVLITE)*(1. + UVLITE)
       DRATE= KDCOMP*(1. + UVLITE)*(1. + UVLITE)
C  BACKWARD DIFFERENCE INTEGRATION OF CZ EQUATION--REQUIRES
C    ALGEBRAIC MANIPULATIONS.
          D1= GMOLES*(1.-XYZ)/V
          D2= 1./TAU
          D3= 0.
      IF(TOC .GT. 0.0) D3= ALPHA*RATE*TOC*ETOC
      IF(CZ.GT.0.0) GO TO 10
       AECOZ= 0.
       BECOZ= 0.
       AEOZD= 0.
       BEOZD= 0.
      GO TO 20
   10   CONTINUE
C  APPROXIMATIONS RESULTING FROM FIRST ORDER TAYLOR
C   SERIES EXPANSION
       AECOZ= (1.-ECOZ)*CZ**ECOZ
       BECOZ= ECOZ*CZ**(ECOZ-1.)
       AEOZD= (1.-EOZD)*CZ**EOZD
       BEOZD= EOZD*CZ**(EOZD-1.)
   20 CONTINUE
```

```
          D4=  (D1*ZIN + D2*CZIN - D3*AECOZ - DRATE*AEOZD) *DT
          D5= -(D1/AUX + D2 + D3*BECOZ + DRATE*BEOZD) *DT
      CZNEW=(CZ+D4)/(1.-D5)
       ZTOP=ZIN*XYZ+(1.0-XYZ)*CZNEW/AUX
C   CALCULATE TIME DERIVATIVE OF OZONE CONCENTRATION
          DCZ=  (CZNEW-CZ)/DT
      TCREAC= 0.
      IF(TOC .GT. 0.0) TCREAC= RATE*(TOC**ETOC)*(CZ**ECOZ)
C   CALCULATE TIME DERIVATIVE OF TOC CONCENTRATION
         DTOC=  (TOCIN-TOC)/TAU - TCREAC
      TOCRCT= TOCRCT + TCREAC*V*DT
        ZOUT= ZTOP
C DETERMINE IF ANY OUTPUT IS NECESSARY AT THIS STEP
      IF(NWRITE .LE. 0) GO TO 50
       JWRITE= JWRITE + 1
      IF(JWRITE .LT. NWRITE) GO TO 50
   30 CONTINUE
      JWRITE= 0
      WRITE(6,40) ZIN, CZIN, TOCIN, G, F, ZOUT, AREA, CZOUT,
     &          TOCOUT, V, CZ, TOC, TAU, GMOLES, ZUX, XYZ,
     &          RATE, DRATE, UVLITE, TCREAC, DCZ, DTOC, DT,
     &          D1, D2, D3, D4, D5, AECOZ, BECOZ, AEOZD,
     &          BECZD ,CZNEW
   40 FORMAT(' IN USTAGE',(/1X,8E12.4))
   50 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE HC
C
C  THIS IS THE HYPOCHLORINATION INTERFACE
C
C                      ___________________
C       CALCIUM       |                   |
C     HYPOCHLORITE    | HYPOCHLORINATION  | EFFLUENT
C     ------------>   |                   |------------> 2
C         FEED        |       UNIT        | (OUTPUT)
C   1 ------------>   |___________________|
C
C  PARAMETER        QUANTITY
C      1            pH OF THE OUTPUT
C      2            INITIAL CHLORITE IN THE HC UNIT
C      3            INITIAL TSS CONC.
C      4            INITIAL TDS CONC.
C      5            INITIAL TOC CONC.
C      6            FEED RATE OF CALCIUM HYPOCHLORITE
C      7            VOLUME OF HYPOCHLORINATION UNIT
C      8            CONC. OF CAOCL2 FEED
C
C  THE FEED STREAM MUST BE SPECIFIED FIRST
C  THE EFFLUENT STREAM MUST BE SPECIFIED SECOND
      REAL*8 HOCLD, CCLD, PH1, F1, FIN, V, ALPHA, RD, KEQ,
     &       CAOCL2, PHI, HCCLI, OCLI, CLI, FAC
      REAL MWHOCL, MWOCL
      COMMON /HCSAV2/ MWHOCL, MWOCL, RHO
      COMMON /MATBAL/ BALNCE(4), AMTIN(4), AMTOUT(4)
      COMMON /CTIME/  TIME, FTIME, DT
      COMMON STREAM(4,100), ICONFG(8,100), PAR(500), NPAR,
     &       NCALL, IUNIT, NFATER, NS, NEQ, DESC(5)
      COMMON /HCSAVE/ PHI, HOCLI, OCLI
      COMMCN /HCPARM/V, ALPHA, RD, KEQ, CAOCL2, JWRITE, MCNT
      COMMON /HCSTOR/ SS, DS, TOC
      COMMON /MATDIS/ MATCAL
         FIN= PAR(NPAR+5)
           V= PAR(NPAR+6)
      CAOCL2= PAR(NPAR+7)
      IF(NCALL) 10,70,80
   10    PHI= PAR(NPAR)
      IF(MATCAL .NE. 0) GO TO 20
          SS= PAR(NPAR+2)
          DS= PAR(NPAR+3)
         TOC= PAR(NPAR+4)
         FAC= PAR(NPAR+1)
        OCLI= (FAC*RHO/1000000.)/((10.**(-PHI)/KEQ)*
     &                                MWHOCL+MWOCL)
       HOCLI= (OCLI*10.**(- PHI))/KEQ
   20 CCNTINUE
      BALNCE(1)= BALNCE(1)  + V
      BALNCE(2)= BALNCE(2)  + V*SS
      BALNCE(3)= BALNCE(3)  + V*DS
      BALNCE(4)= BALNCE(4)  + V*TOC
```

```
      IF(ICONFG(3,IUNIT) .GT. 0) GO TO 40
      WRITE(6,30) IUNIT, ICCNFG(3,IUNIT)
   30  FORMAT(6X,'**** ERROR, UNIT',I5,' FIRST STREAM IN',
     & 'CONFIGURATION IS',I5,'. MUST BE THE FEED.')
      NFATER= NFATER + 1
   40   IF(ICONFG(4,IUNIT) .LT. 0) GO TO 60
      WRITE(6,50)IUNIT,ICONFG(4,IUNIT)
   50 FORMAT(6X,'**** ERROR, UNIT',I5,'. SECOND STREAM IN',
     & ' CONFIGURATICN IS',I5,'. MUST BE THE EFFLUENT.')
      NFATER= NFATER + 1
   60  CONTINUE
C  THE HCSS ROUTINE EXPECTS THE TOTAL CHLORINE DEMAND, RD,
C   TO BE EXPRESSED IN MOLAR UNITS. SIMILARLY FOR ALPHA
C
C  AS ENTERED IN THE INPUT DATA, RD IS IN TERMS OF PARTS PER
C   MILLION. ALPHA IS IN TERMS OF FRACTIONAL PARTS PER MILLI
C    THE FOLLOWING SECTION OF CODE RE-COMPUTES ALPHA AND RD
C               A MOLAR BASIS.
       HOCLD= (RD*ALPHA*RHO)/(1000000.*MWHOCL)
        OCLD= (RD*RHO/1000000. - HOCLD*MWHOCL)/MWOCL
          RD= HOCLD + OCLD
       ALPHA= 0.
      IF(RD .GT. 0.) ALPHA= HOCLD/RD
   70 CONTINUE
      RETURN
   80 CONTINUE
       IFEED= ICONFG(3,IUNIT)
       IPROD= -ICONFG(4,IUNIT)
          F1= STREAM(1,IFEED)
         PH1= 7.0
      CALL HCSS(F1,FIN,PH1)
         FAC= (HOCLI*MWHOCL+OCLI*MWOCL)/RHO*1000000.
         DSS= (F1*STREAM(2,IFEED) - (F1+FIN)*SS)/V
         DDS= (F1*STREAM(3,IFEED) - (F1+FIN)*DS)/V
        DTOC= (F1*STREAM(4,IFEED) - (F1+FIN)*TOC)/V
          SS= SS + DSS*DT
          DS= DS + DDS*DT
         TOC= TOC + DTOC*DT
      STREAM(1,IPROD)= F1 + FIN
      STREAM(2,IPROD)= SS
      STREAM(3,IPROD) = DS
      STREAM(4,IPROD) = TOC
      PAR(NPAR+1)= FAC
      PAR(NPAR)= PHI
      RETURN
      END
```

```
      SUBROUTINE HCSS(F1,FIN,PH1)
C
C THIS SUBROUTINE PERFORMS THE STEADY STATE HYPOCHLORINATION
C   CALCULATIONS
C SEE THE REPORT BY SMITH AND STARKS ON THE HC UNIT FOR A
C   DISCRIPTION OF VARIABLES
C
      REAL*8 V, ALPHA, RD, KEQ, CAOCL2, PHI, HOCLI, OCLI,
     &        H1, H, OH, OH1, F1, F2, PH1, FIN, SUM, DSUM,
     &        HOCLBG, HOCLSM, HOCL, OCL, HOCLP, ATERM,
     &        BTERM, CTERM, X, RADCL, HNEW
      COMMON /HCPARM/V, ALPHA, RD, KEQ, CAOCL2, JWRITE, MCNT
      COMMON /HCSAVE/ PHI, HOCLI, OCLI
      COMMON /CTIME/ TIME, FTIME, DT
      EQUIVALENCE (JERROR,JWRITE)
      DATA JERRCT/0/
          H1= 10.0**(-PH1)
           H= 10.0**(-PHI)
         OH1= 1.E-14/H1
          OH= 1.E-14/H
          F2= F1 + FIN
C  BEGIN SOLUTION
         SUM= HOCLI + OCLI
        DSUM= (2.*FIN*CAOCL2-F1*RD-F2*SUM)/V
         SUM= SUM + DSUM*DT
      HOCLBG= SUM
      HOCLSM= 0.0
      DO 60 I= 1, MCNT
        HOCL= (HOCLBG+HOCLSM)/2.
C  ATERM, BTERM, AND CTERM ARE THE COEFFICIENTS USED IN THE
C       SOLUTION OF X
        ATERM= H + (F1*H1 + 2.*FIN*CAOCL2 - F2*HOCL -
     &             F2*H - ALPHA*RD*F1)*DT/V
        BTERM= -F2*DT/V
        CTERM= OH+ (F1*OH1+2.*FIN*CAOCL2-F2*OH)*DT/V
        RADCL= ((CTERM + ATERM)*(CTERM + ATERM) -
     &          4.0*(ATERM*CTERM - 1.E-14))
      IF(RADCL .GE. 0.0) GO TO 10
C  HOCL IS TOO SMALL
      GO TO 20
   10   CONTINUE
           X= (-(CTERM+ATERM)+DSQRT(RADCL))/2./BTERM
        HNEW=   ATERM+BTERM*X
C  CHECK FOR UNREALISTIC VALUES OF H+ AT TIME T+DT
        IF(HNEW.LE.0.0) GO TO 30
          OCL= KEQ*HOCL/HNEW
C  DETERMINE HOCL', THE CHECK ON ASSUMED VALUE OF HOCL
        HOCLP= SUM-OCL
      IF(HOCL .GT. HOCLP) GO TO 30
   20 HOCLSM= HOCL
      GO TO 40
   30 HOCLBG= HOCL
   40 CONTINUE
```

```
      IF(JERROR .LE. 0) GO TO 60
C   DETERMINE IF ANY WRITING IS TO BE PERFORMED
      JERRCT= JERRCT + 1
      IF(JERRCT .LT. JERROR) GO TO 60
      WRITE(6,50)  I, TIME, HOCL, HOCLP, OCL, HNEW, X, RADCL,
     &             ATERM, BTERM, CTERM, HOCLBG, HOCLSM, H, OH
   50 FORMAT(' IN HYPOCL...I= ',I5,(/1X,5G15.5))
   60 CONTINUE
C   UPDATE VALUES TO TIME T+DT
       HOCLI= HOCL
        OCLI= OCL
         PHI= -DLOG10(HNEW)
      RETURN
      END
```

```
      SUBROUTINE SK
C
C  SIMULATION OF STREAM SINK
C
C                       -------------
C          INPUT       |             |
C         STREAMS      |             |
C     1-5 --------->   |    SINK     |
C                      |             |
C                      |_____________|
C
C  THERE ARE NO PARAMETERS
      COMMON /LOOK/ ISW
      COMMON STREAM(4,100), ICONFG(8,100), PAR(500), NPAR,
     &       NCALL, IUNIT, NFATER, NS, NEQ, DESC(5)
      COMMON /MATBAL/ BALNCE(4), AMTIN(4), AMTOUT(4)
      COMMON /CTIME/  TIME, FTIME, DT
C  ASCERTAIN IF READ DATA, INITIALIZE OR SIMULATE
      IF(NCALL) 10, 20, 30
C  RETURN IF MATERIAL BALANCE CALCULATIONS
   10 RETURN
C  THERE ARE NO INITIALIZATION CALCULATIONS
   20 RETURN
C  SIMULATE CALCULATIONS CONSIST ONLY OF MATERIAL BALANCE
C    EQUATIONS
   30 DO 50 I=3,7
           J=ICONFG(I,IUNIT)
      IF(J .EQ. 0) GO TO 60
           F= STREAM(1,J)
      AMTOUT(1)= AMTOUT(1)  + F*DT
      DO 40 L=2,4
   40 AMTOUT(L)= AMTOUT(L)  + F*STREAM(L,J) *DT
   50 CONTINUE
   60 IF(ISW.EQ.1) WRITE(6,70) (AMTOUT(I),I=1,4)
   70 FORMAT(' UNIT',I5,' SK  TOTALS  FLOW=', G10.3,5X,
     & 'SS=',G10.3,5X,'DS=',G10.3,5X,'TOC=',G10.3)
      RETURN
      END
```

```
      SUBROUTINE SENSOR
C
C  THIS SUBROUTINE SENSES A UNIT PARAMETER OR A STREAM
C    ELEMENT AND PRODUCES THE TIME INTEGRAL OF THE ERROR
C
C
C                          ___________
C        MEASURED         |           |   OUTPUT
C      * * * * * * >|  SENSOR   |* * * * * * * >
C          VALUE          |           | (TO CONTROLLER)
C                         |___________|
C
C  PARAMETER          QUANTITY
C      1              UNIT OR STREAM NUMBER
C      2              PARAMETER OR ELEMENT NUMBER
C      3              INITIAL OUTPUT VALUE
C      4              INTEGRATION TIME CONSTANT, TAU
C    IF TAU IS EQUAL TO ZERO, THEN THE VALUE IS RETURNED
C    IF TAU IS NON-ZERO, THEN
C          (NEW VALUE - OLD OUTPUT VALUE)/TAU
C      IS INTEGRATED AS THE NEW OUTPUT VALUE
      COMMON /LOOK/  ISW
      DATA IGET/'G'/
      COMMON STREAM(4,100), ICONFG(8,100), PAR(500), NPAR,
     &       NCALL, IUNIT, NPATER, NS, NEQ, DESC(5)
      COMMON /CTIME/ TIME, FTIME, DT
      IF(NCALL) 10,20,30
C  NO MATERIAL BALANCE CALCULATIONS
   10 RETURN
   20 CONTINUE
   30 CONTINUE
           I= PAR(NPAR)
           J= PAR(NPAR+1)
      CALL GETPUT(IGET,I,J,R)
           C= PAR(NPAR+2)
         TAU= PAR(NPAR+3)
      IF(TAU.EQ.0.0) GOTO50
          DC= (R-C)/TAU
      IF(ISW .GT. 0)
     & WRITE(6,40) I, J, C, TAU, DC, C, R
   40 FORMAT(' IN SENSOR ',(8G15.5,/1X))
           C= C + DC*DT
      GO TO 60
   50      C= R
   60 PAR(NPAR+2)=C
      RETURN
      END
```

```
      SUBROUTINE MANIP
C
C THIS SUBROUTINE IS USED TO CHANGE THE VALUE OF A PARAMETER
C   OF A UNIT, IE. INCREASE A PUMP OR AN OVERFLOW FLOW RATE
C
C
C                                  ______________
C          VALUE         |                      |  CONTROLLED
C    * * * * * * * * * >| MANIPULATOR |* * * * * * * >
C    (FROM CONTROLLOR) |                       |  PARAMETER
C                         |______________|
C
C  PARAMETER        QUANTITY
C      1            NUMBER OF UNIT TO MANIPULATE (NEGATIVE)
C      2            PARAMETER NUMBER
C      3            OUTPUT VALUE
C      4            UPPER LIMIT
C      5            LOWER LIMIT
      REAL LOVAL
      COMMON /LOOK/  ISW
      DATA IPUT/'P'/
      COMMON STREAM(4,100), ICONFG(8,100), PAR(500), NPAR,
     &       NCALL, IUNIT, NFATER, NS, NEQ, DESC(5)
      IF(NCALL) 10,20,30
   10 RETURN
   20 CONTINUE
   30 CONTINUE
        ITEM= PAR(NPAR)
      IF(ITEM .LT. 0) GO TO 50
      WRITE(6,40) ITEM, IUNIT
   40 FORMAT(' IN ROUTINE MANIP...CAN ONLY MANIPULATE',
     & ' EQUIPMENT....YOU HAVE SPECIFIED STREAM NUMBER',I10,
     & '. CURRENT UNIT NUMBER IS',I10)
      NFATER= NFATER + 1
   50 CONTINUE
           J= PAR(NPAR+1)
       VALUE= PAR(NPAR+2)
       HIVAL= PAR(NPAR+3)
       LOVAL= PAR(NPAR+4)
      IF(VALUE .GT. HIVAL) VALUE= HIVAL
      IF(VALUE .LT. LOVAL) VALUE= LOVAL
      IF(ISW .GT. 0)
     & WRITE(6,60) ITEM, J, VALUE, HIVAL, LOVAL
   60 FORMAT(' IN MANIP ', (8G15.5,/1X))
      PAR(NPAR+2)= VALUE
      CALL GETPUT(IPUT,ITEM,J,VALUE)
      RETURN
      END
```

```
      SUBROUTINE BINARY
C
C  THIS SUBROUTINE IS USED TO SIMULATE A BINARY CONTROLLER
C
C
C                           ______________
C        FROM              |              |       TO
C     * * * * * * * >|   BINARY     |* * * * * * * * >
C       SENSOR             |  CONTBOLLER  | MANIPULATOR
C                          |______________|
C
C  PARAMETER          CCNTENT
C     1               SENSOB NUMBER
C     2               MANIPULATOR NUMBER
C     3               LOWER SET POINT VALUE
C     4               UPPER SET POINT VALUE
C     5               VALUE OF THE CONTROLLED VARIABLE
C     6               UPPER LIMIT OUTPUT VALUE
C     7               LOWER LIMIT OUTPUT VALUE
C     8               OPERATION MODE (NEGATIVE= AUTOMATIC,
C                     POSITIVE= OUTPUT VALUE FOR MANUAL MODE)
      REAL LOWSET,LOVAL
      COMMON STREAM(4,100), ICONFG(8,100), PAR(500), NPAR,
     &       NCALL, IUNIT, NFATER, NS, NEQ, DESC(5)
      COMMCN/LOCK/ISW
      DATA IGET, IPUT/'G', 'P'/
      IF(NCALL) 10, 20, 30
   10 RETURN
   20 CONTINUE
   30 CONTINUE
         ISEN= PAR(NPAR)
         IMAN= PAR(NPAR+1)
       LOWSET= PAR(NPAR+2)
        HISET= PAR(NPAR+3)
        VALUE= PAR(NPAR+4)
        HIVAL= PAR(NPAR+5)
        LOVAL= PAR(NPAR+6)
        AMODE= PAR(NPAR+7)
      IF(AMODE .GT. 0.) GO TO 60
C  CONTROLLER IS ON AUTO
      CALL GETPUT(IGET,ISEN,3,VNEW)
      IF(VNEW .GT. LOWSET .AND. VNEW .GT. HISET) VALUE= HIVAL
      IF(VNEW .LT. LOWSET .AND. VNEW .LT. HISET) VALUE= LOVAL
   40  CALL GETPUT(IPUT,IMAN,3,VALUE)
      IF(ISW.GT.0)
     & WRITE(6,50) ISEN, IMAN, LOWSET, LOVAL, HIVAL, AMODE,
     &             VNEW, VALUE
   50 FORMAT(' IN BINARY ', (8G15.5,/1X))
      PAR(NPAR+4)= VALUE
      RETURN
C  CONTBOLLER IS ON MANUAL
   60  VALUE= AMODE
      GO TO 40
      END
```

```
      SUBROUTINE RATIO
C
C   THIS SUBROUTINE SIMULATE A RATIO CONTROLLER
C
C                            _____________
C                           |             |
C    FROM SENSOR       |    RATIO      | TO MANIPULATOR
C    * * * * * * >| CONTROLLER |* * * * * * * * >
C                           |_____________|
C
C   PARAMETER          QUANTITY
C       1              SENSOR UNIT NUMBER
C       2              MANIPULATOR UNIT NUMBER
C       3              RATIO
C       4              OPERATION MODE (NEGATIVE= AUTOMATIC
C                      POSITIVE= OUTPUT VALUE FOR MANUAL)
C
      REAL M
      COMMON STREAM(4,100), ICONFG(8,100), PAR(500), NPAR,
     &       NCALL, IUNIT, NFATER, NS, NEQ, DESC(5)
      COMMON /LOCK/  ISW
      DATA IPUT, IGET/'P', 'G'/
      IF(NCALL) 10, 20, 30
   10 RETURN
   20 CONTINUE
   30 CONTINUE
        ISEN= PAR(NPAR)
        IMAN= PAR(NPAR+1)
      CALL GETPUT(IGET,ISEN,3,C)
           R= PAR(NPAR+2)
       AMODE= PAR(NPAR+3)
      IF(AMODE .GT. 0) GO TO 60
           M= R*C
      IF(ISW .GT. 0)
     & WRITE(6,40) ISEN, IMAN, R, C, AMODE, M
   40 FORMAT(' IN RATIO ',(8G15.5,/1X))
   50 CALL GETPUT(IPUT,IMAN,3,M)
      RETURN
   60      M= AMODE
      GOTO50
      END
```

```
      SUBROUTINE PID
C
C  THIS SUBROUTINE SIMULATES A PID CONTROLLER
C    USING THE VELOCITY ALGORITHM
C
C
C    FROM SENSOR     |-------------| TO MANIPULATOR
C   * * * * * * * * >|    P-I-D    |* * * * * * * * >
C                    |             |
C                    |_____________|
C
C  PARAMETER         QUANTITY
C      1             UNIT NUMBER OF THE SENSOR(NEGATIVE)
C      2             UNIT NUMBER OF THE MANIPULATOR(NEGATIVE)
C      3             SETPOINT
C      4             GAIN
C      5             RESET TIME
C      6             DERIVATIVE TIME
C      7             MODE OF OPERATION (NEGATIVE= AUTOMATIC,
C                    POSITIVE= OUTPUT VALUE FOR MANUAL)
C
      REAL KC,M
      COMMON STREAM(4,100), ICONFG(8,100), PAR(500), NPAR,
     &       NCALL, IUNIT, NFATER, NS, NEQ, DESC(5)
      COMMON /CTIME/  TIME, FTIME, DT
      COMMON /PIDSAV/ EIM1, EIM2
      COMMON /LOOK/   ISW
      DATA IGET, IPUT/'G', 'P'/
C  THIS ROUTINE USES THE VELOCITY ALGORITHM
        ISEN= PAR(NPAR)
        IMAN= PAR(NPAR+1)
      IF(NCALL) 10,20,40
   10 RETURN
C  CHECK TO SEE IF ACCESSING SENSORS AND MANIPULATORS
  20    EIM1= 0.
        EIM2= 0.
      IF(IMAN .LT. 0 .AND. ISEN .LT. 0) GO TO 40
      WRITE(6,30) IMAN, ISEN
   30 FORMAT(' IN PID...IMPROPERLY SPECIFIED SENSOR OR ',
     & ' MANIPULATOR'/' MANIPULATOR IS',I5,' SENSOR IS',I5)
      NFATER= NFATER + 1
      RETURN
  40       R= PAR(NPAR+2)
      CALL GETPUT(IGET,ISEN,3,C)
          EI= R - C
          KC= PAR(NPAR+3)
          TI= PAR(NPAR+4)
          TD= PAR(NPAR+5)
       AMODE= PAR(NPAR+6)
      IF(AMODE .GT. 0.) GO TO 60
C  CONTROLLER IS ON AUTO
          DE= (EI - EIM1)/DT
         DE2= (EI - 2.*EIM1 + EIM2)/(DT*DT)
```

```
          DM= KC*(DE + EI/TI + TD*DE2)
      CALL GETPUT(IGET,IMAN,3,M)
      IF(ISW .GT. 0)
     & WRITE(6,50) ISEN, IMAN, R, C, EI, EIM1, EIM2, KC,
     &              TI, TD, AMODE, DE, DE2, DM, M
   50 FORMAT(' IN PID ',(8G15.5,/1X))
          M= M + DM*DT
      CALL GETPUT(IPUT,IMAN,3,M)
        EIM2= EIM1
        EIM1= EI
      RETURN
C   CONTROLLER IS ON MANUAL
   60     M= AMODE
      CALL GETPUT(IPUT,IMAN,3,M)
      RETURN
      END
```

```
      SUBROUTINE GETPUT(ICODE,ITEMO,J,VALUE)
C
C  THIS SUBROUTINE PROVIDES THE INTERFACE BETWEEN THE
C  SENSORS AND CONTROLLERS AND THE PROCESS UNITS AND STREAMS
C  IF ICODE= 'P' THEN "VALUE" IS ASSIGNED TO THE PARAMETER
C   OR ELEMENT SPECIFIED BY "ITEMO" AND "J"
C  IF ICODE= 'G' THEN "VALUE" IS SET EQUAL TO THE VALUE
C   OF THE SPECIFIED PARAMETER OR ELEMENT
C  ITEMO= UNIT NUMBER IF NEGATIVE
C       = STREAM NUMBER IF POSITIVE
C  J= UNIT PARAMETER OR STREAM ELEMENT NUMBER
C
      COMMON STREAM(100,4), ICONFG(100,8), PAR(500), NPAR,
     &       NCALL, IUNIT, NFATER, NS, NEQ, DESC(5)
      COMMON /LOOK/  ISW
      DATA IPUT/'P'/
      DATA IGET/'G'/
        ITEM= ITEMO
C     CHECK ON VALIDITY OF ICODE
      IF(ICODE .EQ. IGET .OR. ICODE .EQ. IPUT) GO TO 20
      WRITE(6,10) ICODE
   10 FORMAT(' IN ROUTINE GETPUT...INVALID CODE.',/' ICODE',
     & ' IN I FORMAT IS ',I10,' ICODE IN A FORMAT IS ',A1)
      NFATER= NFATER + 1
      RETURN
   20 IF(ITEM .GT. 0) GO TO 60
C  HAVE A PIECE OF EQUIPMENT
        ITEM= -ITEM
C  FIND POSITION "K" OF UNIT IN CONFIGURATION
C   (POSITION IS NOT NECESSARILY EQUAL TO THE UNIT NUMBER)
      DO 30 K=1,NEQ
      IF(ICONFG(K,1) .EQ. ITEM) GO TO 50
   30 CONTINUE
      WRITE(6,40) ITEM
   40 FORMAT(' IN ROUTINE GETPUT...UNABLE TO FIND UNIT'
     &,' NUMBER',I5,/'  SETTING ERROR CODE')
      NFATER= NFATER + 1
      RETURN
C  HAVE FOUND CORRECT PIECE OF EQUIPMENT
   50      N= ICONFG(K,8)
C  N= LOCATION OF FIRST PARAMETER FOR THIS UNIT IN "PAR"
      IF(ICODE .EQ. IPUT) PAR(N+J-1)= VALUE
      IF(ICODE .EQ. IGET) VALUE= PAR(N+J-1)
      RETURN
C  WE HAVE A STREAM
   60 IF(ICODE .EQ. IGET) VALUE= STREAM(ITEM,J)
      IF(ICODE .EQ. IPUT) STREAM(ITEM,J)= VALUE
      GO TO 50
      END
```

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